Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +) -5.97 ±0.89 (n=49)
logP (neutral X) 3.14 ±0.01 (n=49)

18B-28012 Points 1 to 30

M07_octanol concentration factor 0.885
Carbonate 0.0000 mM
Acidity error 0.24941 mM

18B-28012 Points 31 to 62

M07_octanol concentration factor 0.786
Carbonate 0.0623 mM
Acidity error 0.05292 mM

18B-28012 Points 63 to 95

M07_octanol concentration factor 0.842
Carbonate 0.0998 mM
Acidity error 0.05919 mM

Warnings and errors

Errors None
Warnings One or more logP values out of range

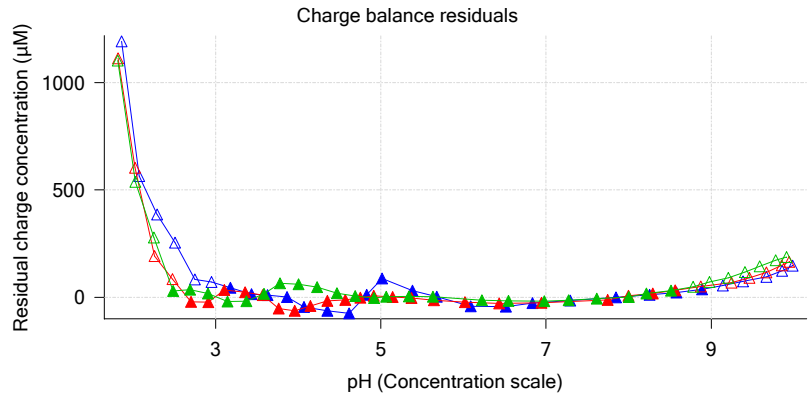
Sample logD and percent species

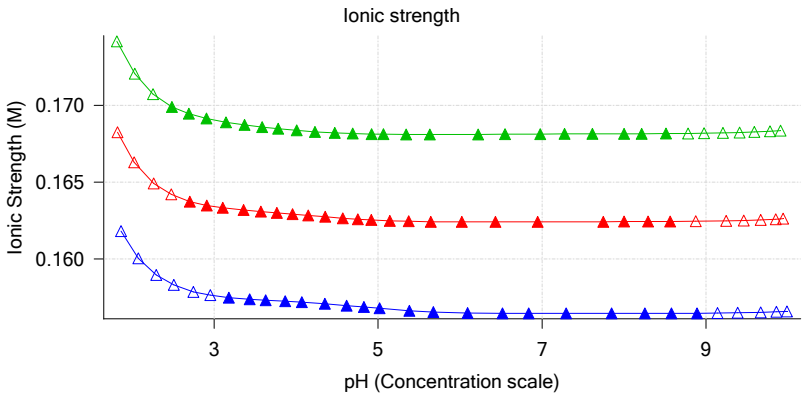
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	-1.93	98.83 %	0.00 %	0.00 %	1.16 %	
1.200	-1.73	98.17 %	0.00 %	0.00 %	1.83 %	Stomach pH
2.000	-0.93	89.45 %	0.01 %	0.00 %	10.54 %	
3.000	0.07	45.89 %	0.04 %	0.00 %	54.07 %	
4.000	1.07	7.82 %	0.07 %	0.00 %	92.12 %	
5.000	2.04	0.84 %	0.07 %	0.00 %	99.09 %	
6.000	2.80	0.08 %	0.07 %	0.00 %	99.84 %	
6.500	3.00	0.03 %	0.07 %	0.00 %	99.90 %	
7.000	3.09	0.01 %	0.07 %	0.00 %	99.92 %	
7.400	3.12	0.00 %	0.07 %	0.00 %	99.92 %	Blood pH
8.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
9.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
10.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
11.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	
12.000	3.14	0.00 %	0.07 %	0.00 %	99.93 %	

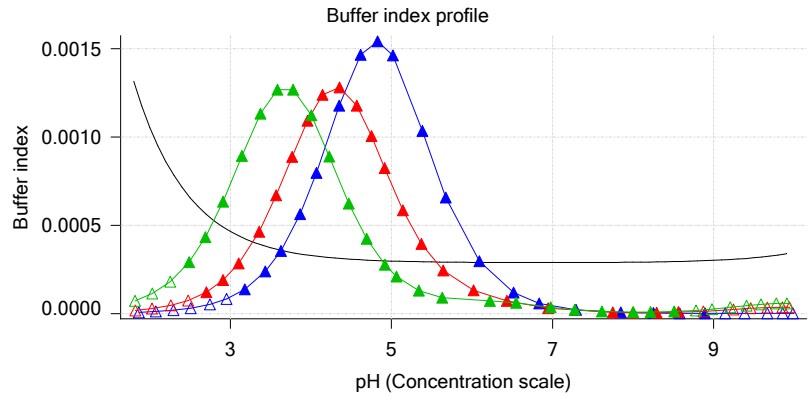
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

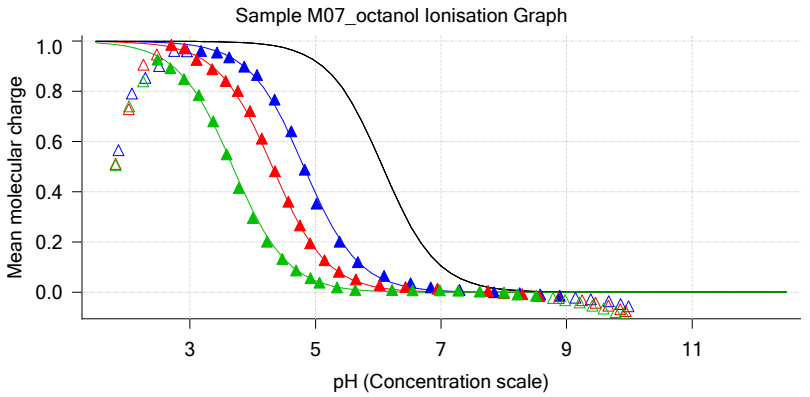
Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

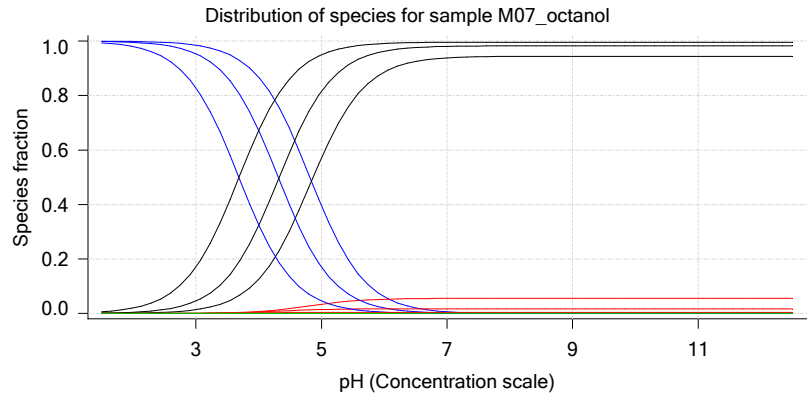
Graphs

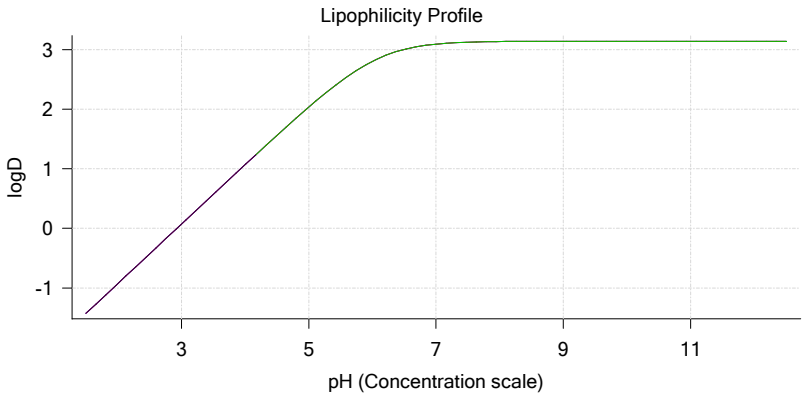


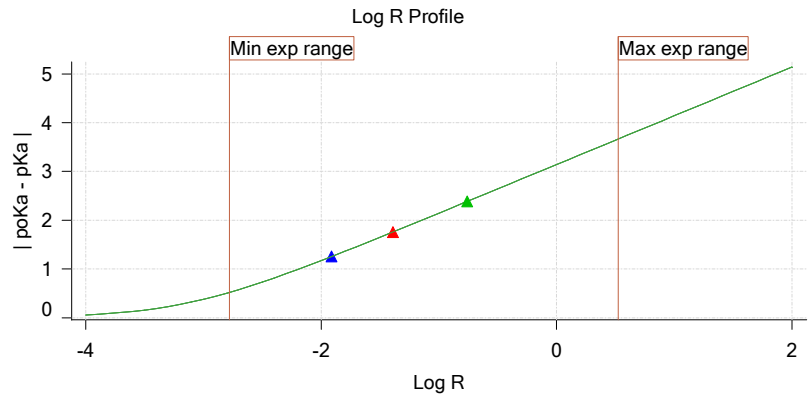


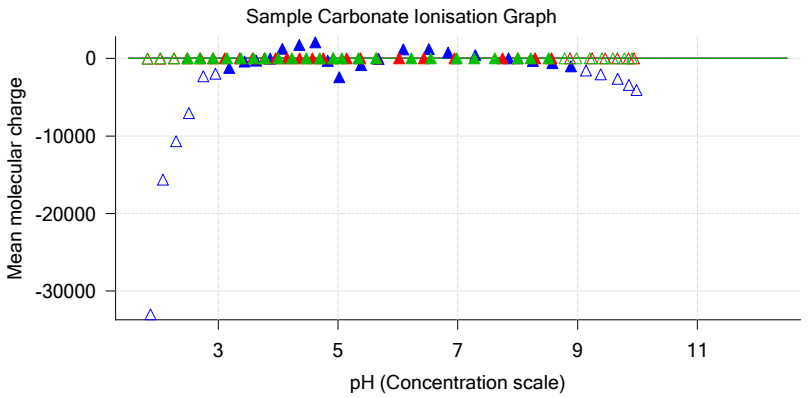








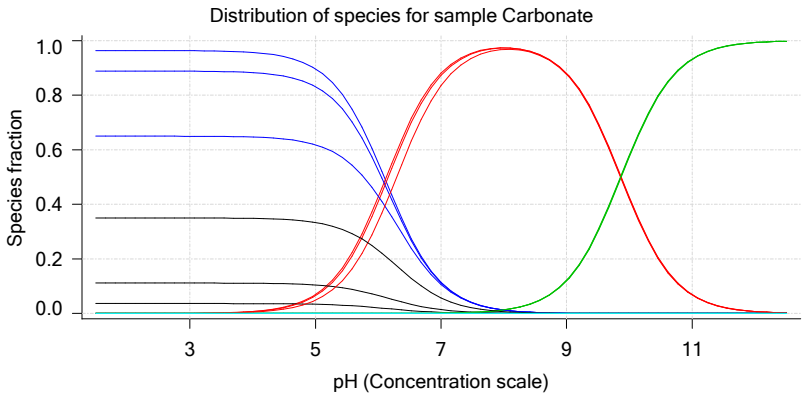




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M07_octanol**	Experiment start time:	**2/28/2018 5:44:56 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28012**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18B-28012 Points 1 to 30

Overall results

RMSD	0.538
Average ionic strength	0.157 M
Average temperature	25.0°C
Partition ratio	0.0122 : 1
Analyte concentration range	2983.5 µM to 3075.2 µM
Total points considered	19 of 30

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r

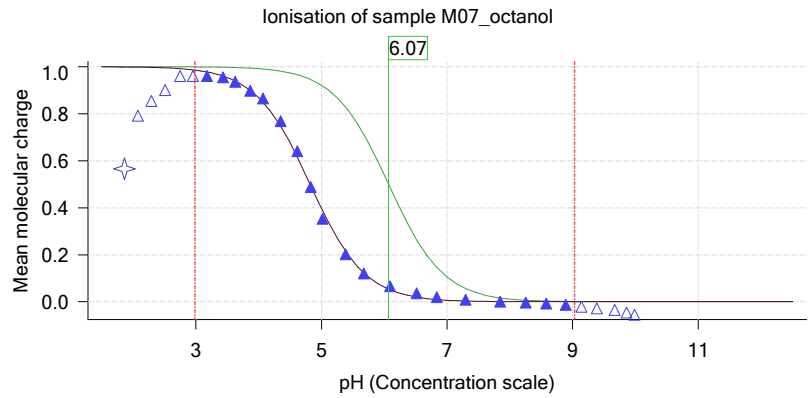
Titrants

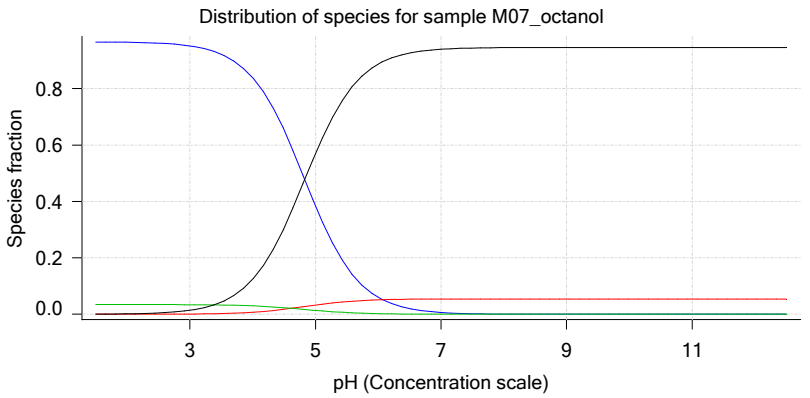
0.50 M HCl	0.993513	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 5:44:56 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M07_octanol concentration factor	0.885
Base pKa 1	6.07
logP (XH +)	0.46
logP (neutral X)	3.15

Sample graphs

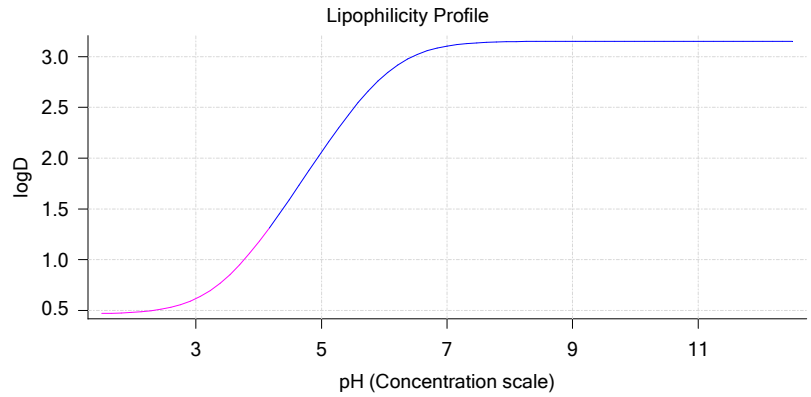




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



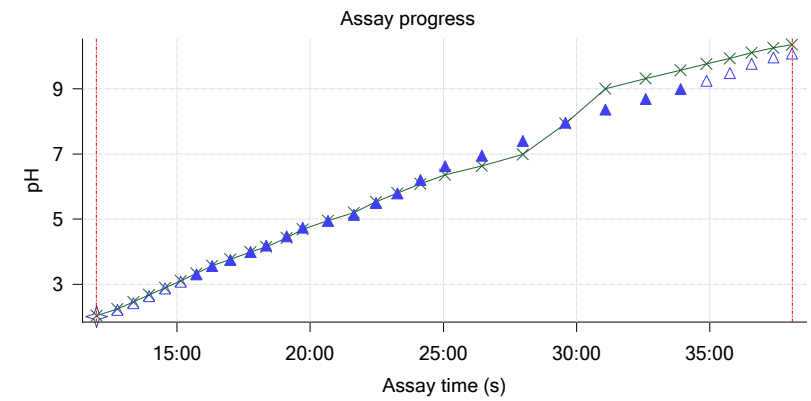
Sample logD and percent species

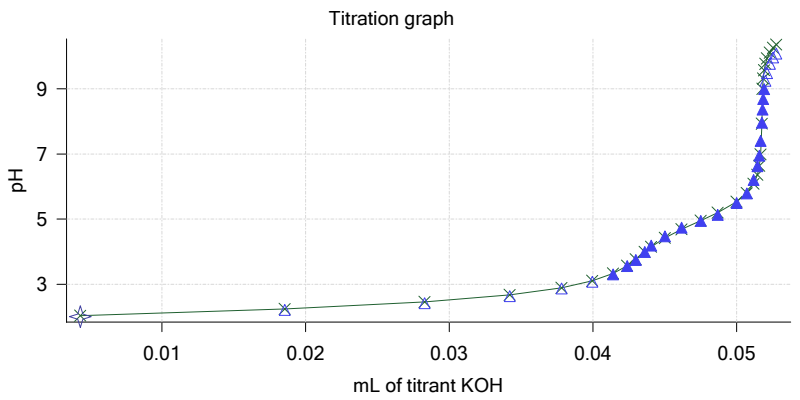
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.46	96.55 %	0.00 %	3.43 %	0.01 %	
1.200	0.47	96.55 %	0.00 %	3.43 %	0.02 %	Stomach pH
2.000	0.48	96.42 %	0.01 %	3.43 %	0.14 %	
3.000	0.61	95.13 %	0.08 %	3.38 %	1.41 %	
4.000	1.17	83.88 %	0.71 %	2.98 %	12.42 %	
5.000	2.06	38.44 %	3.27 %	1.37 %	56.92 %	
6.000	2.82	5.99 %	5.10 %	0.21 %	88.70 %	
6.500	3.02	1.98 %	5.32 %	0.07 %	92.63 %	
7.000	3.10	0.63 %	5.40 %	0.02 %	93.94 %	
7.400	3.13	0.25 %	5.42 %	0.01 %	94.32 %	Blood pH
8.000	3.15	0.06 %	5.43 %	0.00 %	94.50 %	
9.000	3.15	0.01 %	5.43 %	0.00 %	94.56 %	
10.000	3.15	0.00 %	5.44 %	0.00 %	94.56 %	
11.000	3.15	0.00 %	5.44 %	0.00 %	94.56 %	
12.000	3.15	0.00 %	5.44 %	0.00 %	94.56 %	

Carbonate and acidity

Carbonate 0.000 mM
Acidity error 0.249 mM

Other graphs

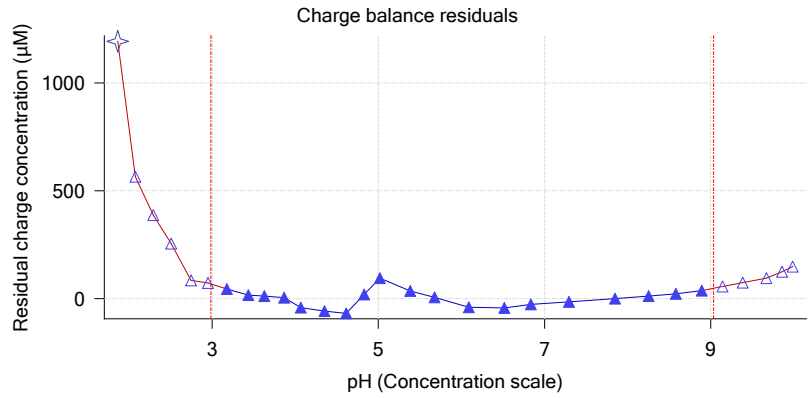


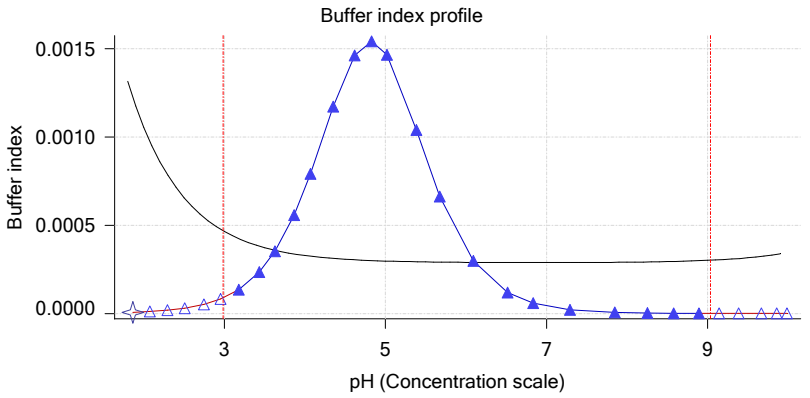


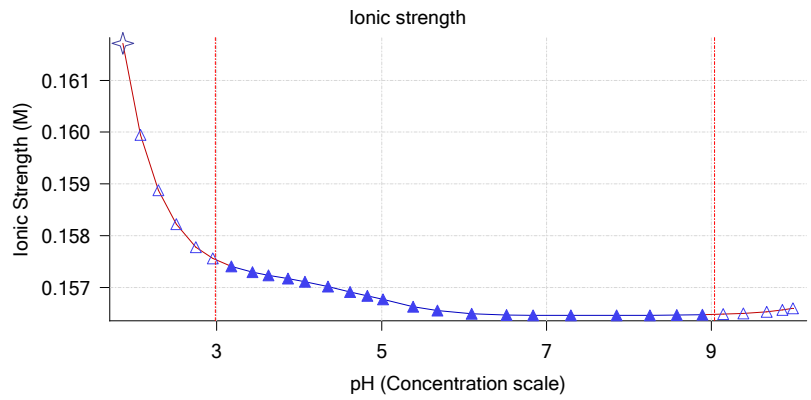
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

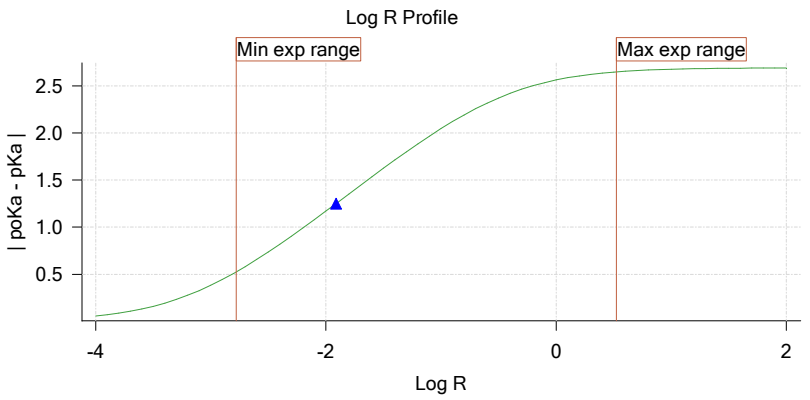
Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

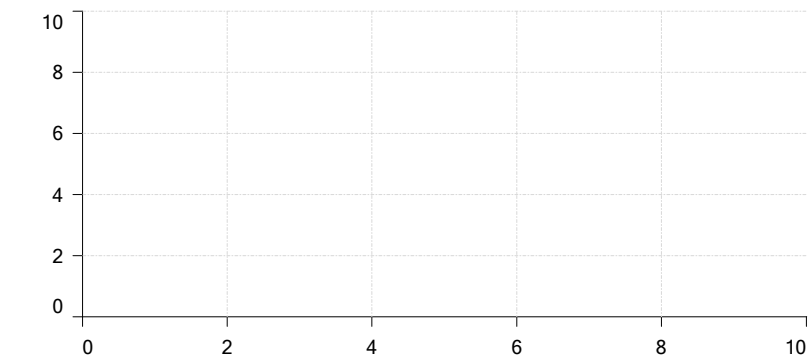
Other graphs (continued)

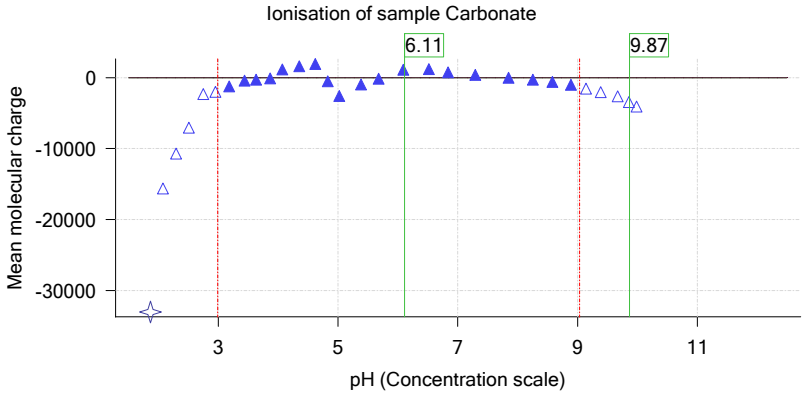












Sample name:	**M07_octanol**	Experiment start time:	**2/28/2018 5:44:56 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28012**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18B-28012 Points 31 to 62

Overall results

RMSD	0.578
Average ionic strength	0.163 M
Average temperature	25.0°C
Partition ratio	0.0406 : 1
Analyte concentration range	2713.2 µM to 2800.4 µM
Total points considered	22 of 32

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r

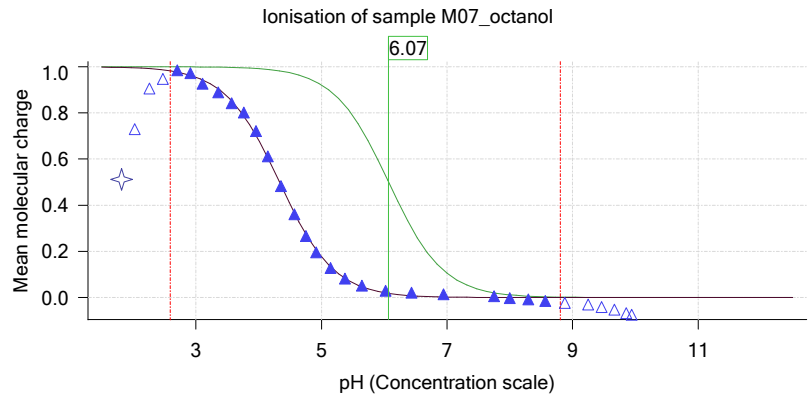
Titrants

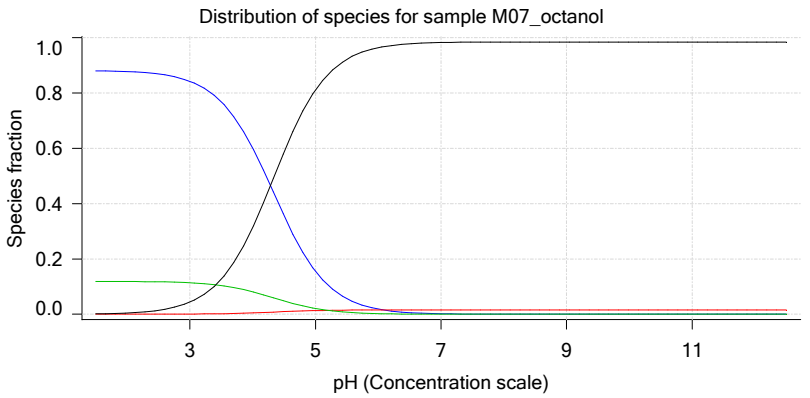
0.50 M HCl	0.993513	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 5:44:56 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M07_octanol concentration factor	0.786
Base pKa 1	6.07
logP (XH +)	0.52
logP (neutral X)	3.18

Sample graphs

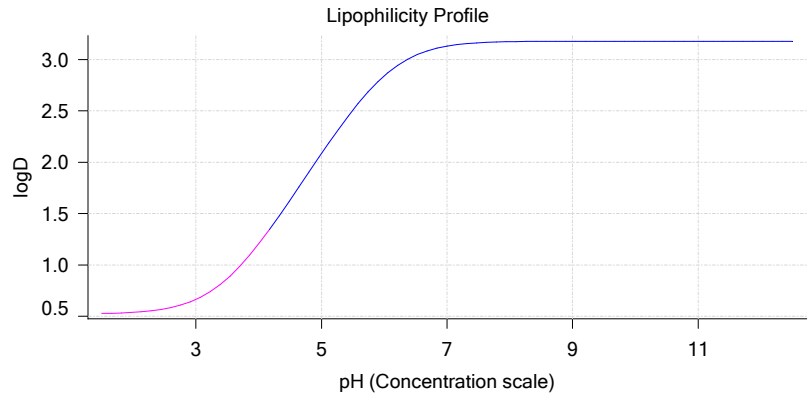




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



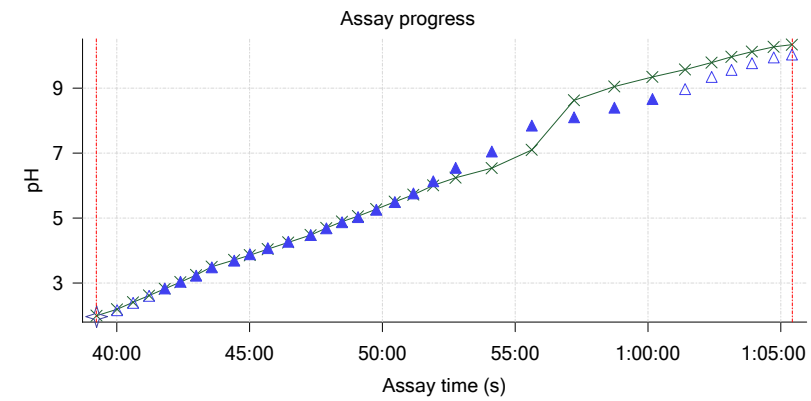
Sample logD and percent species

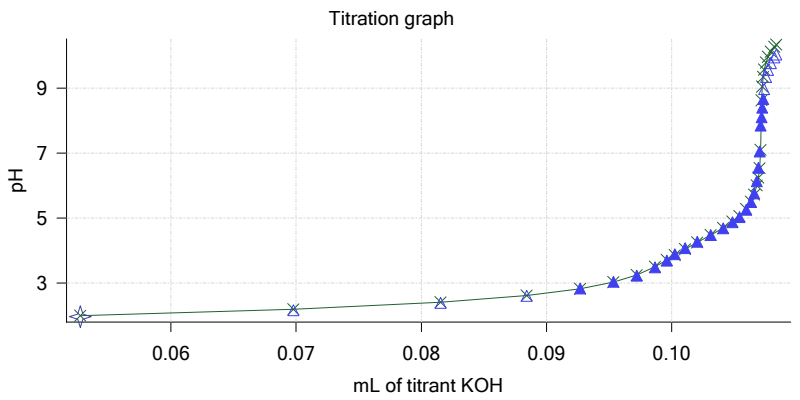
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.52	88.06 %	0.00 %	11.89 %	0.05 %	
1.200	0.52	88.04 %	0.00 %	11.89 %	0.07 %	Stomach pH
2.000	0.54	87.69 %	0.01 %	11.84 %	0.46 %	
3.000	0.66	84.18 %	0.07 %	11.37 %	4.38 %	
4.000	1.20	60.09 %	0.51 %	8.11 %	31.29 %	
5.000	2.08	15.56 %	1.32 %	2.10 %	81.02 %	
6.000	2.84	1.85 %	1.57 %	0.25 %	96.33 %	
6.500	3.04	0.59 %	1.60 %	0.08 %	97.73 %	
7.000	3.13	0.19 %	1.60 %	0.03 %	98.18 %	
7.400	3.16	0.08 %	1.61 %	0.01 %	98.31 %	Blood pH
8.000	3.17	0.02 %	1.61 %	0.00 %	98.37 %	
9.000	3.18	0.00 %	1.61 %	0.00 %	98.39 %	
10.000	3.18	0.00 %	1.61 %	0.00 %	98.39 %	
11.000	3.18	0.00 %	1.61 %	0.00 %	98.39 %	
12.000	3.18	0.00 %	1.61 %	0.00 %	98.39 %	

Carbonate and acidity

Carbonate 0.062 mM
Acidity error 0.053 mM

Other graphs

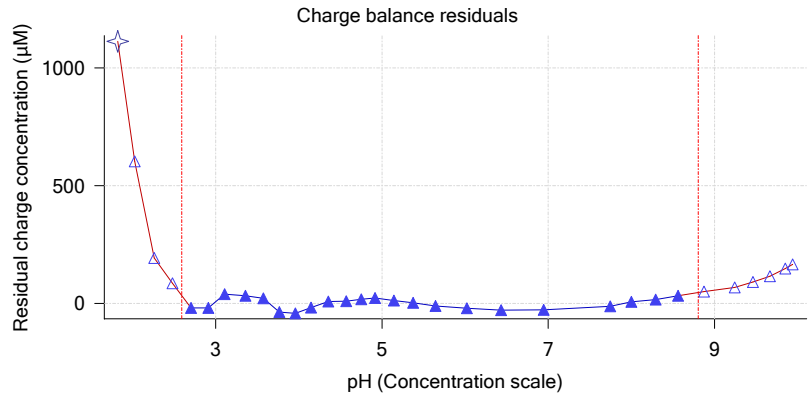


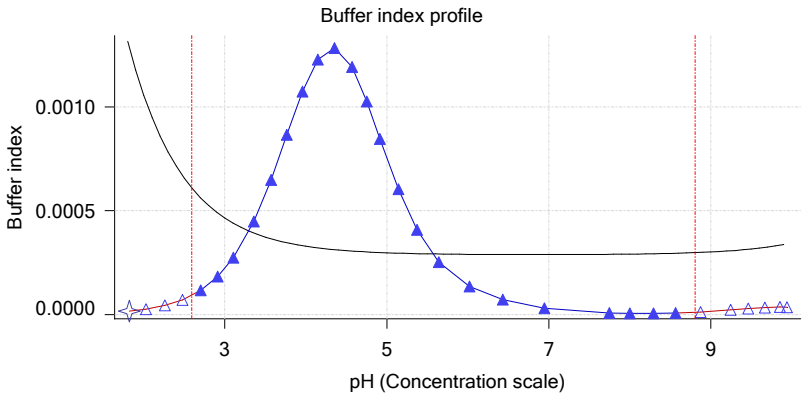


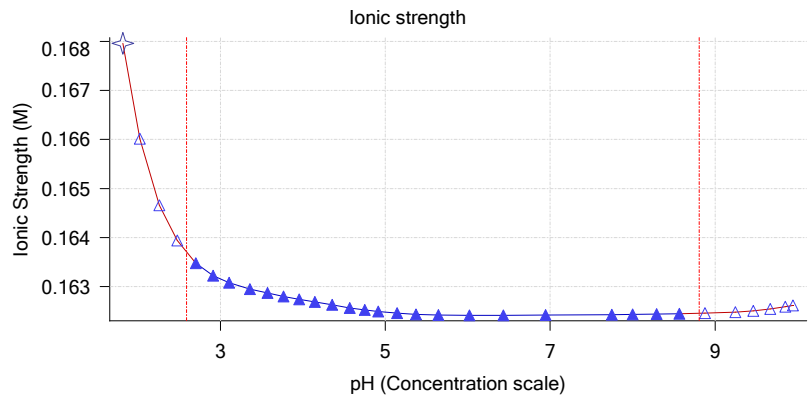
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

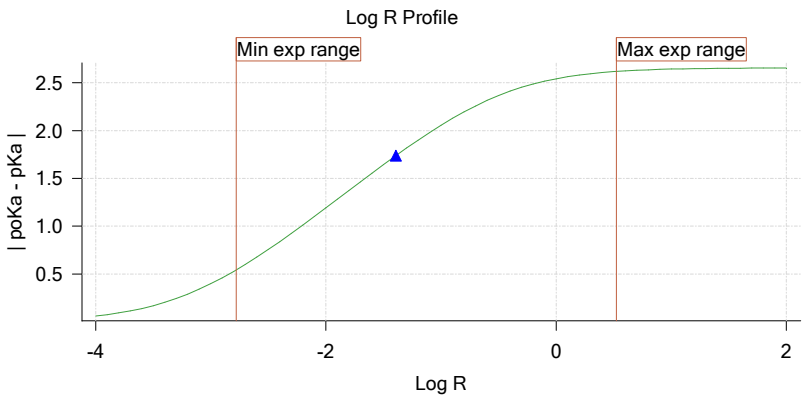
Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

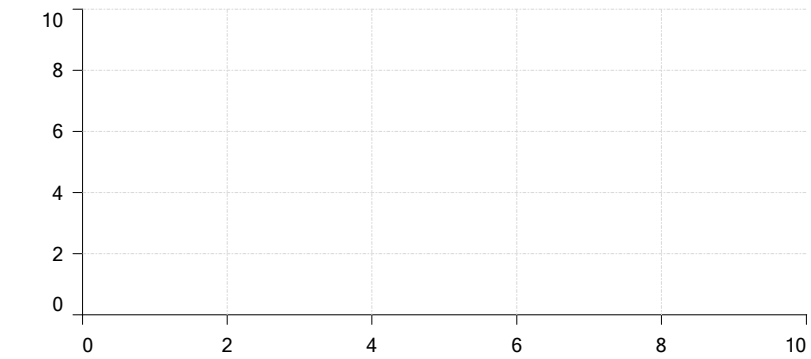
Other graphs (continued)

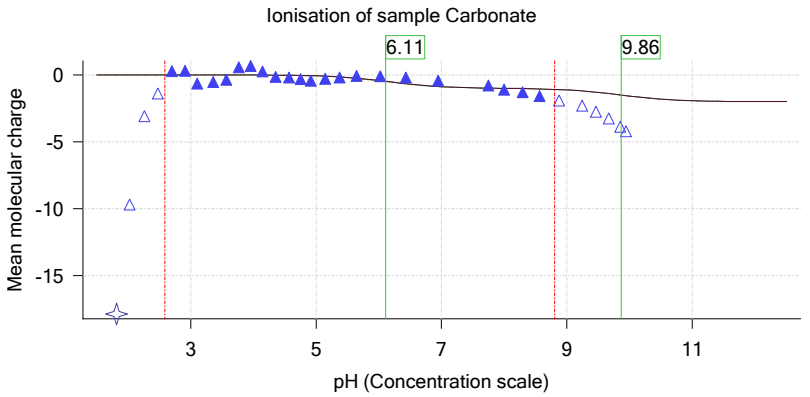












Sample name:	**M07_octanol**	Experiment start time:	**2/28/2018 5:44:56 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28012**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18B-28012 Points 63 to 95

Overall results

RMSD	0.432
Average ionic strength	0.168 M
Average temperature	25.0°C
Partition ratio	0.1744 : 1
Analyte concentration range	2246.9 µM to 2311.5 µM
Total points considered	23 of 33

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r

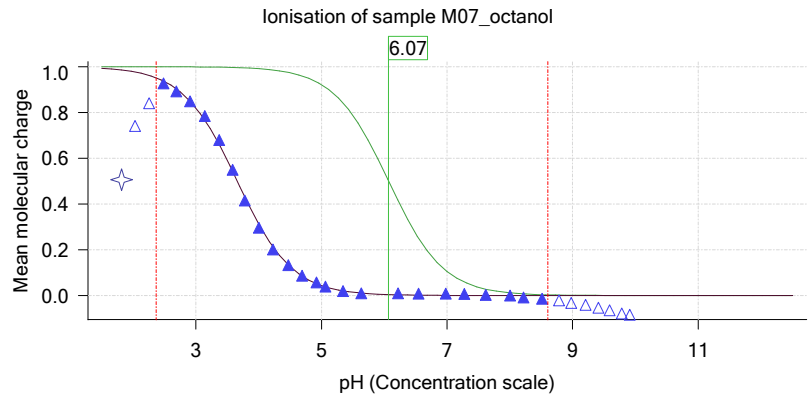
Titrants

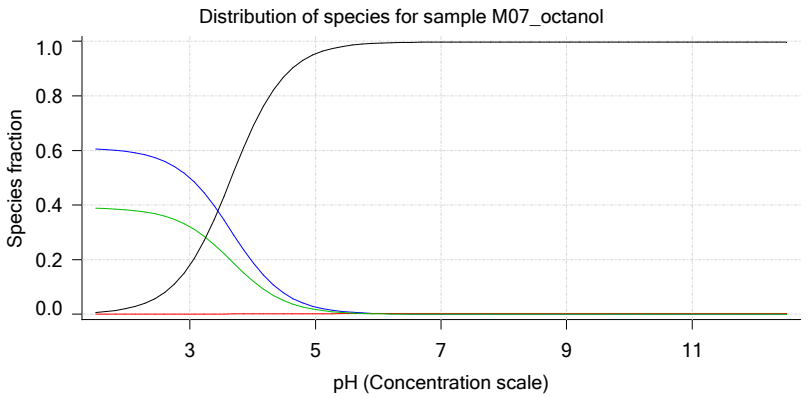
0.50 M HCl	0.993513	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 5:44:56 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M07_octanol concentration factor	0.842
Base pKa 1	6.07
logP (XH +)	0.57
logP (neutral X)	3.38

Sample graphs

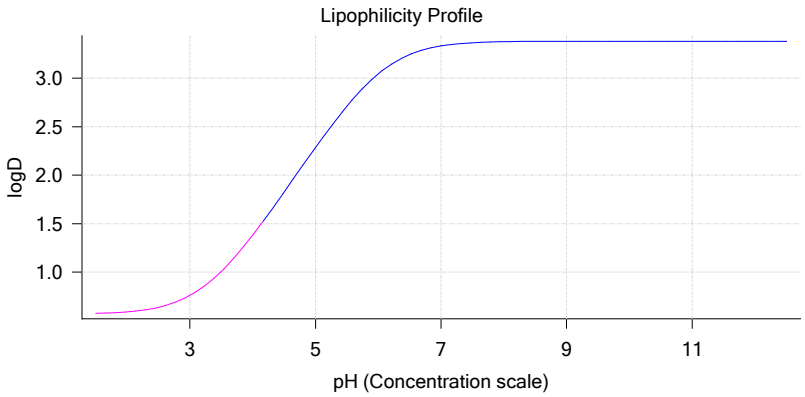




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



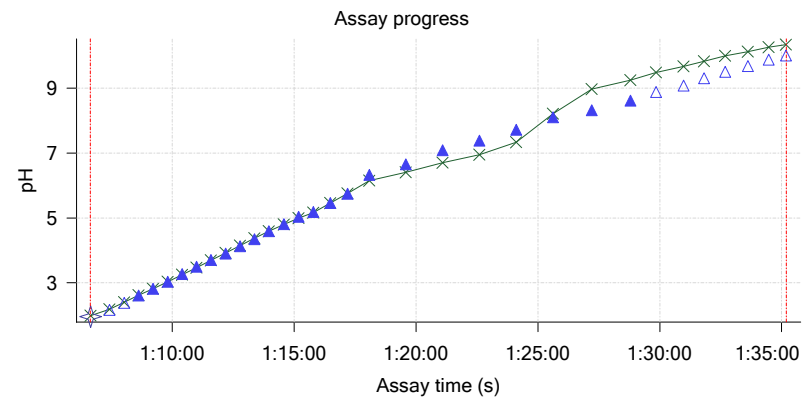
Sample logD and percent species

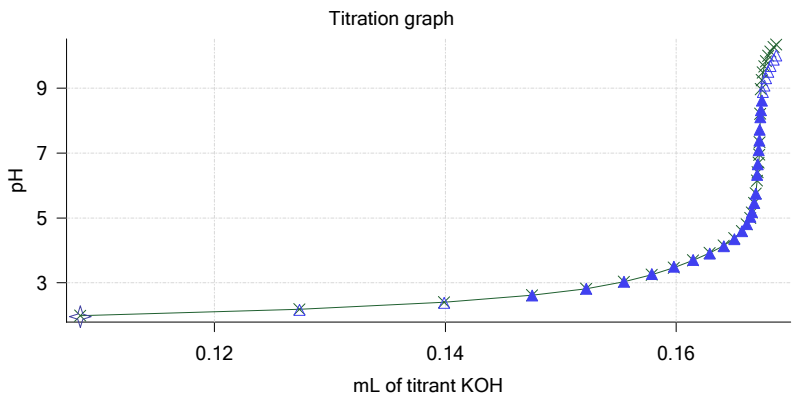
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.57	60.78 %	0.00 %	39.00 %	0.22 %	
1.200	0.57	60.70 %	0.00 %	38.95 %	0.34 %	Stomach pH
2.000	0.59	59.61 %	0.01 %	38.25 %	2.14 %	
3.000	0.76	49.98 %	0.04 %	32.07 %	17.91 %	
4.000	1.38	19.11 %	0.16 %	12.26 %	68.47 %	
5.000	2.28	2.66 %	0.23 %	1.71 %	95.40 %	
6.000	3.05	0.28 %	0.24 %	0.18 %	99.31 %	
6.500	3.25	0.09 %	0.24 %	0.06 %	99.62 %	
7.000	3.33	0.03 %	0.24 %	0.02 %	99.72 %	
7.400	3.36	0.01 %	0.24 %	0.01 %	99.74 %	Blood pH
8.000	3.38	0.00 %	0.24 %	0.00 %	99.76 %	
9.000	3.38	0.00 %	0.24 %	0.00 %	99.76 %	
10.000	3.38	0.00 %	0.24 %	0.00 %	99.76 %	
11.000	3.38	0.00 %	0.24 %	0.00 %	99.76 %	
12.000	3.38	0.00 %	0.24 %	0.00 %	99.76 %	

Carbonate and acidity

Carbonate 0.100 mM
Acidity error 0.059 mM

Other graphs

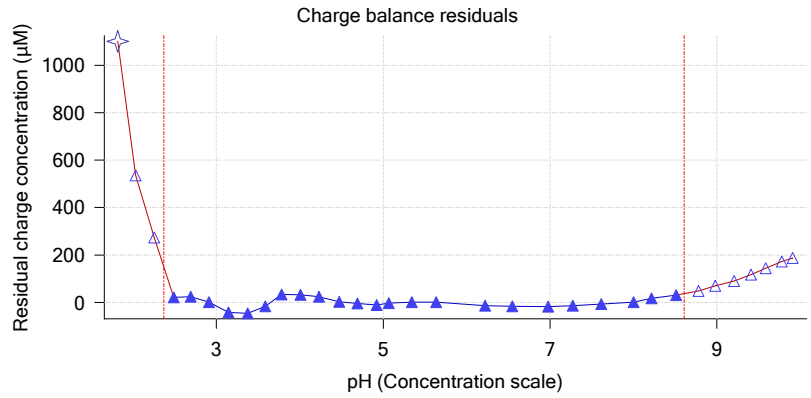


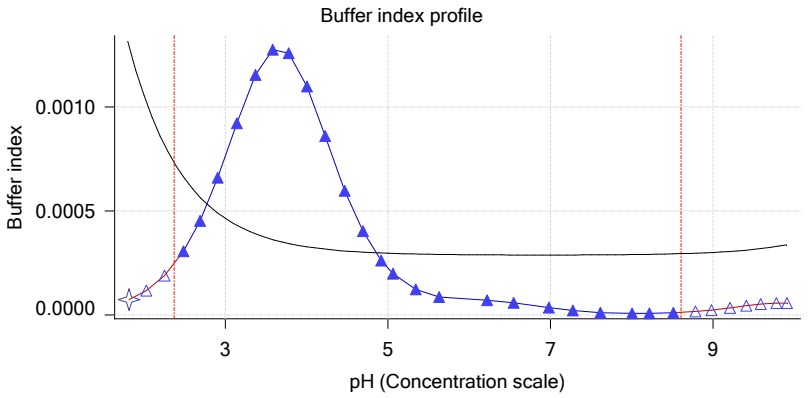


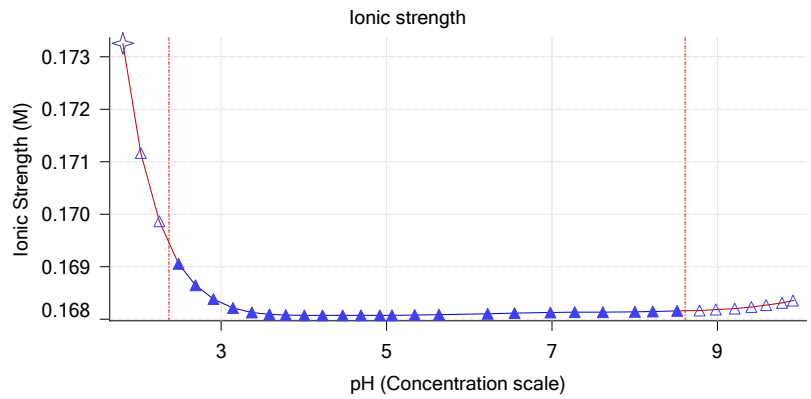
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

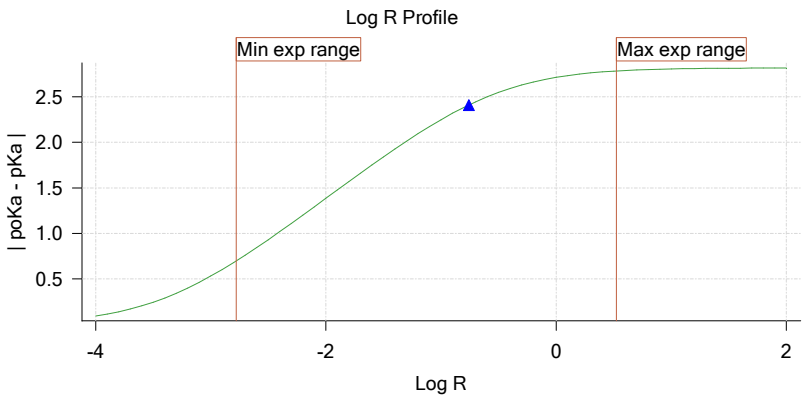
Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

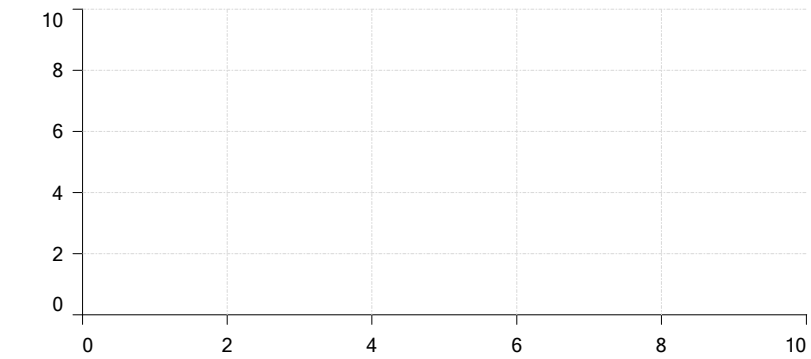
Other graphs (continued)

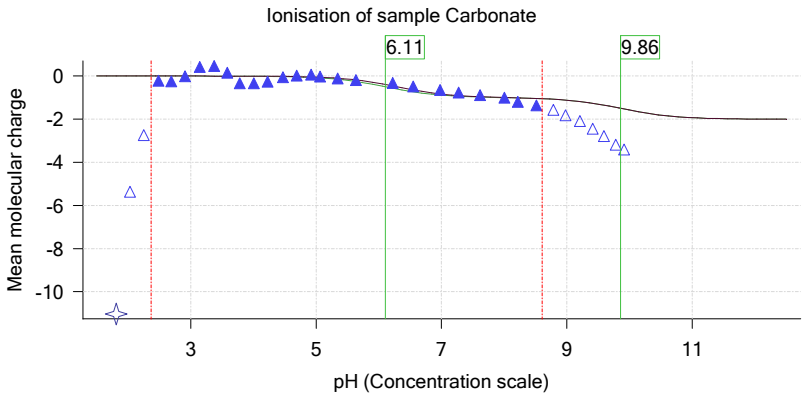












Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M07_octanol	2/27/2018 4:29:24 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001140 g	2/28/2018 4:24:13 PM	User entered value
Formula weight	235.28 g/mol	2/27/2018 4:29:24 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	235.28	2/27/2018 4:29:24 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:29:24 PM	User entered value
Sample is a	Base	2/27/2018 4:29:24 PM	User entered value
pKa 1	6.07	2/27/2018 4:29:24 PM	User entered value
logp (XH +)	0.50	2/28/2018 1:33:04 PM	User entered value
logP (neutral X)	3.44	2/28/2018 1:33:10 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
8:59.8	Initial pH = 8.94									
11:59.4	Data point 1	1.50000 mL	0.05127 mL	0.00433 mL	0.01999 mL	1.999	-0.00679	0.88781	0.00036	10.5 s
12:46.0	Data point 2	1.50000 mL	0.05127 mL	0.01856 mL	0.01999 mL	2.206	-0.00488	0.10282	0.00075	10.0 s
13:21.7	Data point 3	1.50000 mL	0.05127 mL	0.02829 mL	0.01999 mL	2.420	-0.00179	0.10235	0.00028	10.0 s
13:57.3	Data point 4	1.50000 mL	0.05127 mL	0.03420 mL	0.01999 mL	2.634	0.00674	0.36990	0.00055	10.5 s
14:33.3	Data point 5	1.50000 mL	0.05127 mL	0.03782 mL	0.01999 mL	2.871	-0.00703	0.23966	0.00071	10.0 s
15:08.8	Data point 6	1.50000 mL	0.05127 mL	0.03996 mL	0.01999 mL	3.075	-0.00875	0.22861	0.00090	10.0 s
15:44.1	Data point 7	1.50000 mL	0.05127 mL	0.04139 mL	0.01999 mL	3.301	-0.00343	0.34132	0.00029	10.0 s
16:19.5	Data point 8	1.50000 mL	0.05127 mL	0.04238 mL	0.01999 mL	3.554	-0.00525	0.72590	0.00030	10.0 s
17:00.2	Data point 9	1.50000 mL	0.05127 mL	0.04297 mL	0.01999 mL	3.748	-0.00822	0.25539	0.00080	10.0 s
17:45.9	Data point 10	1.50000 mL	0.05127 mL	0.04360 mL	0.01999 mL	3.985	0.00207	0.02036	0.00072	10.0 s
18:21.3	Data point 11	1.50000 mL	0.05127 mL	0.04405 mL	0.01999 mL	4.187	-0.00914	0.64694	0.00056	10.0 s
19:07.1	Data point 12	1.50000 mL	0.05127 mL	0.04501 mL	0.01999 mL	4.469	-0.01050	0.85079	0.00056	10.5 s
19:43.0	Data point 13	1.50000 mL	0.05127 mL	0.04617 mL	0.01999 mL	4.732	-0.00875	0.19263	0.00099	11.0 s
20:40.1	Data point 14	1.50000 mL	0.05127 mL	0.04751 mL	0.01999 mL	4.944	-0.00471	0.06280	0.00093	12.5 s
21:38.6	Data point 15	1.50000 mL	0.05127 mL	0.04868 mL	0.01999 mL	5.133	-0.01539	0.58584	0.00099	13.5 s
22:27.9	Data point 16	1.50000 mL	0.05127 mL	0.05000 mL	0.01999 mL	5.497	-0.01785	0.90166	0.00093	18.0 s
23:16.5	Data point 17	1.50000 mL	0.05127 mL	0.05071 mL	0.01999 mL	5.789	-0.01719	0.91631	0.00089	21.0 s
24:08.1	Data point 18	1.50000 mL	0.05127 mL	0.05118 mL	0.01999 mL	6.202	-0.01867	0.95635	0.00094	25.0 s
25:03.7	Data point 19	1.50000 mL	0.05127 mL	0.05143 mL	0.01999 mL	6.626	-0.01776	0.83266	0.00096	47.5 s
26:26.9	Data point 20	1.50000 mL	0.05127 mL	0.05158 mL	0.01999 mL	6.945	-0.01819	0.87488	0.00096	56.5 s
27:59.1	Data point 21	1.50000 mL	0.05127 mL	0.05167 mL	0.01999 mL	7.402	-0.04008	0.97402	0.00201	Timed out at 59.5 s
29:34.7	Data point 22	1.50000 mL	0.05127 mL	0.05174 mL	0.01999 mL	7.954	-0.04746	0.99119	0.00236	Timed out at 59.5 s
31:05.2	Data point 23	1.50000 mL	0.05127 mL	0.05179 mL	0.01999 mL	8.360	-0.02983	0.96268	0.00150	Timed out at 59.5 s
32:35.7	Data point 24	1.50000 mL	0.05127 mL	0.05183 mL	0.01999 mL	8.683	-0.01860	0.94531	0.00095	43.0 s
33:54.3	Data point 25	1.50000 mL	0.05127 mL	0.05191 mL	0.01999 mL	8.994	-0.01985	0.97488	0.00099	28.0 s
34:52.9	Data point 26	1.50000 mL	0.05127 mL	0.05200 mL	0.01999 mL	9.245	-0.01948	0.97749	0.00097	22.0 s
35:45.4	Data point 27	1.50000 mL	0.05127 mL	0.05212 mL	0.01999 mL	9.487	-0.01908	0.98282	0.00095	18.0 s
36:34.0	Data point 28	1.50000 mL	0.05127 mL	0.05230 mL	0.01999 mL	9.769	-0.01911	0.95487	0.00097	13.5 s
37:23.1	Data point 29	1.50000 mL	0.05127 mL	0.05254 mL	0.01999 mL	9.959	-0.01930	0.93400	0.00099	11.0 s
38:04.7	Data point 30	1.50000 mL	0.05127 mL	0.05275 mL	0.01999 mL	10.086	-0.01735	0.90522	0.00090	10.5 s
39:14.5	Data point 31	1.50000 mL	0.10745 mL	0.05275 mL	0.06999 mL	1.956	-0.00499	0.33277	0.00043	10.0 s
40:00.8	Data point 32	1.50000 mL	0.10745 mL	0.06978 mL	0.06999 mL	2.157	-0.00137	0.09377	0.00022	10.0 s
40:36.5	Data point 33	1.50000 mL	0.10745 mL	0.08154 mL	0.06999 mL	2.389	0.01008	0.68241	0.00060	10.5 s
41:12.6	Data point 34	1.50000 mL	0.10745 mL	0.08843 mL	0.06999 mL	2.603	-0.00003	0.00007	0.00018	10.0 s
41:48.1	Data point 35	1.50000 mL	0.10745 mL	0.09269 mL	0.06999 mL	2.825	-0.00269	0.22934	0.00028	10.0 s
42:23.5	Data point 36	1.50000 mL	0.10745 mL	0.09537 mL	0.06999 mL	3.033	-0.00407	0.55814	0.00027	10.0 s
42:58.9	Data point 37	1.50000 mL	0.10745 mL	0.09722 mL	0.06999 mL	3.227	-0.00358	0.59751	0.00023	10.0 s

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
43:34.4	Data point 38	1.50000 mL	0.10745 mL	0.09868 mL	0.06999 mL	3.478	-0.00403	0.43861	0.00030	10.0 s
44:25.3	Data point 39	1.50000 mL	0.10745 mL	0.09962 mL	0.06999 mL	3.690	-0.00498	0.42701	0.00038	10.0 s
45:00.7	Data point 40	1.50000 mL	0.10745 mL	0.10026 mL	0.06999 mL	3.885	-0.00655	0.31183	0.00058	10.0 s
45:41.4	Data point 41	1.50000 mL	0.10745 mL	0.10108 mL	0.06999 mL	4.076	-0.00350	0.03966	0.00087	10.0 s
46:27.2	Data point 42	1.50000 mL	0.10745 mL	0.10205 mL	0.06999 mL	4.264	-0.00534	0.73313	0.00031	10.0 s
47:18.1	Data point 43	1.50000 mL	0.10745 mL	0.10313 mL	0.06999 mL	4.472	-0.00695	0.55723	0.00046	10.0 s
47:53.5	Data point 44	1.50000 mL	0.10745 mL	0.10412 mL	0.06999 mL	4.687	0.00135	0.00555	0.00090	10.0 s
48:28.9	Data point 45	1.50000 mL	0.10745 mL	0.10487 mL	0.06999 mL	4.868	-0.00089	0.00956	0.00045	10.5 s
49:04.9	Data point 46	1.50000 mL	0.10745 mL	0.10543 mL	0.06999 mL	5.032	0.00810	0.39796	0.00063	11.0 s
49:46.4	Data point 47	1.50000 mL	0.10745 mL	0.10597 mL	0.06999 mL	5.258	0.00679	0.13828	0.00090	11.0 s
50:28.0	Data point 48	1.50000 mL	0.10745 mL	0.10635 mL	0.06999 mL	5.487	0.00018	0.00010	0.00089	11.5 s
51:10.0	Data point 49	1.50000 mL	0.10745 mL	0.10661 mL	0.06999 mL	5.756	-0.01673	0.85338	0.00089	14.5 s
51:55.1	Data point 50	1.50000 mL	0.10745 mL	0.10682 mL	0.06999 mL	6.132	-0.01877	0.87402	0.00099	19.5 s
52:45.2	Data point 51	1.50000 mL	0.10745 mL	0.10694 mL	0.06999 mL	6.543	-0.01943	0.92774	0.00100	51.5 s
54:07.2	Data point 52	1.50000 mL	0.10745 mL	0.10703 mL	0.06999 mL	7.054	-0.04976	0.98613	0.00247	Timed out at 59.5 s
55:37.7	Data point 53	1.50000 mL	0.10745 mL	0.10713 mL	0.06999 mL	7.854	-0.06673	0.98909	0.00331	Timed out at 59.5 s
57:13.3	Data point 54	1.50000 mL	0.10745 mL	0.10720 mL	0.06999 mL	8.106	-0.04215	0.99160	0.00209	Timed out at 59.5 s
58:43.8	Data point 55	1.50000 mL	0.10745 mL	0.10724 mL	0.06999 mL	8.397	-0.02007	0.98697	0.00100	50.5 s
1:00:10.1	Data point 56	1.50000 mL	0.10745 mL	0.10731 mL	0.06999 mL	8.669	-0.01679	0.97495	0.00084	38.0 s
1:01:23.7	Data point 57	1.50000 mL	0.10745 mL	0.10741 mL	0.06999 mL	8.978	-0.01933	0.92055	0.00099	29.5 s
1:02:23.8	Data point 58	1.50000 mL	0.10745 mL	0.10755 mL	0.06999 mL	9.347	-0.01767	0.84096	0.00095	14.5 s
1:03:08.8	Data point 59	1.50000 mL	0.10745 mL	0.10771 mL	0.06999 mL	9.564	-0.01365	0.77349	0.00077	15.5 s
1:03:54.9	Data point 60	1.50000 mL	0.10745 mL	0.10793 mL	0.06999 mL	9.768	-0.01979	0.95642	0.00100	13.5 s
1:04:44.1	Data point 61	1.50000 mL	0.10745 mL	0.10821 mL	0.06999 mL	9.953	-0.01717	0.91485	0.00089	10.5 s
1:05:25.1	Data point 62	1.50000 mL	0.10745 mL	0.10837 mL	0.06999 mL	10.042	-0.01543	0.86770	0.00082	10.0 s
1:06:39.2	Data point 63	1.50000 mL	0.16776 mL	0.10837 mL	0.31999 mL	1.951	-0.00886	0.78453	0.00049	10.0 s
1:07:25.4	Data point 64	1.50000 mL	0.16776 mL	0.12737 mL	0.31999 mL	2.161	0.01497	0.60547	0.00095	10.5 s
1:08:01.6	Data point 65	1.50000 mL	0.16776 mL	0.13989 mL	0.31999 mL	2.381	0.00407	0.78143	0.00023	10.0 s
1:08:37.2	Data point 66	1.50000 mL	0.16776 mL	0.14751 mL	0.31999 mL	2.612	0.00821	0.51467	0.00056	10.0 s
1:09:12.7	Data point 67	1.50000 mL	0.16776 mL	0.15221 mL	0.31999 mL	2.814	-0.00211	0.44340	0.00016	10.5 s
1:09:48.8	Data point 68	1.50000 mL	0.16776 mL	0.15548 mL	0.31999 mL	3.031	-0.00824	0.29769	0.00075	10.0 s
1:10:24.3	Data point 69	1.50000 mL	0.16776 mL	0.15788 mL	0.31999 mL	3.265	-0.00300	0.73677	0.00017	10.0 s
1:10:59.7	Data point 70	1.50000 mL	0.16776 mL	0.15981 mL	0.31999 mL	3.493	-0.00479	0.74608	0.00027	10.0 s
1:11:35.2	Data point 71	1.50000 mL	0.16776 mL	0.16148 mL	0.31999 mL	3.705	-0.00484	0.90505	0.00025	10.5 s
1:12:11.2	Data point 72	1.50000 mL	0.16776 mL	0.16291 mL	0.31999 mL	3.900	-0.00806	0.48548	0.00057	10.5 s
1:12:47.1	Data point 73	1.50000 mL	0.16776 mL	0.16414 mL	0.31999 mL	4.124	-0.01087	0.62887	0.00068	10.0 s
1:13:22.5	Data point 74	1.50000 mL	0.16776 mL	0.16505 mL	0.31999 mL	4.346	-0.01000	0.57912	0.00065	10.0 s
1:13:58.0	Data point 75	1.50000 mL	0.16776 mL	0.16571 mL	0.31999 mL	4.587	-0.00486	0.06935	0.00091	11.0 s
1:14:34.4	Data point 76	1.50000 mL	0.16776 mL	0.16613 mL	0.31999 mL	4.808	0.00762	0.26942	0.00072	11.0 s
1:15:10.8	Data point 77	1.50000 mL	0.16776 mL	0.16642 mL	0.31999 mL	5.034	-0.01627	0.71284	0.00095	11.0 s
1:15:47.2	Data point 78	1.50000 mL	0.16776 mL	0.16658 mL	0.31999 mL	5.179	0.01179	0.55572	0.00078	11.5 s
1:16:29.3	Data point 79	1.50000 mL	0.16776 mL	0.16677 mL	0.31999 mL	5.456	-0.00292	0.02167	0.00098	11.5 s
1:17:11.3	Data point 80	1.50000 mL	0.16776 mL	0.16689 mL	0.31999 mL	5.746	-0.01772	0.96453	0.00089	23.5 s
1:18:05.3	Data point 81	1.50000 mL	0.16776 mL	0.16700 mL	0.31999 mL	6.334	-0.01888	0.94530	0.00096	59.0 s
1:19:35.0	Data point 82	1.50000 mL	0.16776 mL	0.16707 mL	0.31999 mL	6.658	-0.04000	0.97540	0.00200	Timed out at 59.5 s
1:21:05.5	Data point 83	1.50000 mL	0.16776 mL	0.16714 mL	0.31999 mL	7.088	-0.06280	0.99503	0.00311	Timed out at 59.5 s
1:22:36.0	Data point 84	1.50000 mL	0.16776 mL	0.16719 mL	0.31999 mL	7.382	-0.07007	0.99379	0.00347	Timed out at 59.5 s
1:24:06.5	Data point 85	1.50000 mL	0.16776 mL	0.16724 mL	0.31999 mL	7.722	-0.06487	0.99756	0.00321	Timed out at 59.5 s
1:25:37.0	Data point 86	1.50000 mL	0.16776 mL	0.16729 mL	0.31999 mL	8.108	-0.04105	0.99278	0.00203	Timed out at 59.5 s

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:27:12.6	Data point 87	1.50000 mL	0.16776 mL	0.16736 mL	0.31999 mL	8.322	-0.02438	0.97344	0.00122	Timed out at 59.5 s
1:28:48.2	Data point 88	1.50000 mL	0.16776 mL	0.16743 mL	0.31999 mL	8.617	-0.01662	0.76643	0.00094	22.0 s
1:29:51.0	Data point 89	1.50000 mL	0.16776 mL	0.16752 mL	0.31999 mL	8.885	-0.01802	0.91131	0.00093	27.0 s
1:30:58.8	Data point 90	1.50000 mL	0.16776 mL	0.16764 mL	0.31999 mL	9.081	-0.01665	0.80009	0.00092	14.5 s
1:31:49.0	Data point 91	1.50000 mL	0.16776 mL	0.16778 mL	0.31999 mL	9.309	-0.01346	0.47170	0.00097	11.5 s
1:32:41.3	Data point 92	1.50000 mL	0.16776 mL	0.16797 mL	0.31999 mL	9.511	-0.01581	0.68192	0.00095	15.0 s
1:33:37.1	Data point 93	1.50000 mL	0.16776 mL	0.16818 mL	0.31999 mL	9.689	-0.00057	0.00339	0.00048	10.5 s
1:34:28.5	Data point 94	1.50000 mL	0.16776 mL	0.16846 mL	0.31999 mL	9.881	-0.01835	0.83849	0.00099	11.5 s
1:35:10.5	Data point 95	1.50000 mL	0.16776 mL	0.16867 mL	0.31999 mL	10.010	0.00024	0.00025	0.00075	10.0 s
1:35:29.7	Assay volumes	1.50000 mL	0.16776 mL	0.16867 mL	0.31999 mL					

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.050 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.250 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	2/28/2018 5:44:56 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	2/28/2018 5:44:56 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+4.52 mV		2/28/2018 5:45:24 PM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Trition X-100 in H20		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.7e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	6.7e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:08] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[8:53] Titrator arm moved to Titration position
[8:53] Argon flow rate set to 100
[8:53] Stirrer speed set to 10
[8:58] Automatically add 0.02000 mL of Octanol
[8:59] Dispensed 0.019991 mL of Octanol
[9:00] Initial pH = 8.94
[9:00] Iterative adjust 8.94 -> 2.00
[9:00] pH 8.94 -> 2.00
[9:02] Air gap released for Acid (0.5 M HCl)
[9:02] Dispensed 0.051270 mL of Acid (0.5 M HCl)
[9:08] Holding pH 2.00
[11:08] Stirrer speed set to 0
[11:08] Stirrer speed set to 50
[11:08] Iterative adjust 1.96 -> 2.00
[11:08] pH 1.96 -> 2.00
[11:08] Air gap released for Base (0.5 M KOH)
[11:09] Dispensed 0.004327 mL of Base (0.5 M KOH)
[12:00] Stirrer speed set to 0
[12:10] Datapoint id 1 collected
[12:10] Stirrer speed set to 50
[12:15] pH 2.01 -> 2.21
[12:15] Using cautious pH adjust
[12:15] Dispensed 0.007808 mL of Base (0.5 M KOH)
[12:21] Stepping pH = 2.10
[12:21] Dispensed 0.005550 mL of Base (0.5 M KOH)
[12:26] Stepping pH = 2.19
[12:26] Dispensed 0.000870 mL of Base (0.5 M KOH)
[12:31] Stepping pH = 2.21
[12:46] Stirrer speed set to 0
[12:56] Datapoint id 2 collected
[12:56] Charge balance equation is out by 8.8%
[12:56] Stirrer speed set to 50

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:01] pH 2.21 -> 2.41
[13:01] Using charge balance adjust
[13:02] Dispensed 0.009737 mL of Base (0.5 M KOH)
[13:22] Stirrer speed set to 0
[13:32] Datapoint id 3 collected
[13:32] Charge balance equation is out by 4.0%
[13:32] Stirrer speed set to 50
[13:37] pH 2.43 -> 2.63
[13:37] Using charge balance adjust
[13:37] Dispensed 0.005903 mL of Base (0.5 M KOH)
[13:57] Stirrer speed set to 0
[14:08] Datapoint id 4 collected
[14:08] Charge balance equation is out by 3.4%
[14:08] Stirrer speed set to 50
[14:13] pH 2.64 -> 2.84
[14:13] Using charge balance adjust
[14:13] Dispensed 0.003622 mL of Base (0.5 M KOH)
[14:33] Stirrer speed set to 0
[14:43] Datapoint id 5 collected
[14:43] Charge balance equation is out by 13.9%
[14:43] Stirrer speed set to 50
[14:49] pH 2.88 -> 3.08
[14:49] Using charge balance adjust
[14:49] Dispensed 0.002140 mL of Base (0.5 M KOH)
[15:09] Stirrer speed set to 0
[15:19] Datapoint id 6 collected
[15:19] Charge balance equation is out by -3.1%
[15:19] Stirrer speed set to 50
[15:24] pH 3.08 -> 3.28
[15:24] Using charge balance adjust
[15:24] Dispensed 0.001435 mL of Base (0.5 M KOH)
[15:44] Stirrer speed set to 0
[15:54] Datapoint id 7 collected
[15:54] Charge balance equation is out by 8.5%
[15:54] Stirrer speed set to 50
[15:59] pH 3.31 -> 3.51
[15:59] Using charge balance adjust
[16:00] Dispensed 0.000988 mL of Base (0.5 M KOH)
[16:20] Stirrer speed set to 0
[16:30] Datapoint id 8 collected
[16:30] Charge balance equation is out by 22.7%
[16:30] Stirrer speed set to 50
[16:35] pH 3.56 -> 3.76
[16:35] Using cautious pH adjust
[16:35] Dispensed 0.000400 mL of Base (0.5 M KOH)
[16:40] Stepping pH = 3.68
[16:40] Dispensed 0.000188 mL of Base (0.5 M KOH)
[16:45] Stepping pH = 3.75
[17:00] Stirrer speed set to 0
[17:10] Datapoint id 9 collected
[17:10] Charge balance equation is out by 25.4%
[17:10] Stirrer speed set to 50
[17:15] pH 3.76 -> 3.96
[17:15] Using cautious pH adjust
[17:16] Dispensed 0.000400 mL of Base (0.5 M KOH)
[17:21] Stepping pH = 3.92
[17:21] Dispensed 0.000071 mL of Base (0.5 M KOH)
[17:26] Stepping pH = 3.93
[17:26] Dispensed 0.000165 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:31] Stepping pH = 3.99
[17:46] Stirrer speed set to 0
[17:56] Datapoint id 10 collected
[17:56] Charge balance equation is out by 18.0%
[17:56] Stirrer speed set to 50
[18:01] pH 4.00 -> 4.20
[18:01] Using cautious pH adjust
[18:01] Dispensed 0.000447 mL of Base (0.5 M KOH)
[18:06] Stepping pH = 4.20
[18:21] Stirrer speed set to 0
[18:32] Datapoint id 11 collected
[18:32] Charge balance equation is out by 50.0%
[18:32] Stirrer speed set to 50
[18:37] pH 4.20 -> 4.40
[18:37] Using cautious pH adjust
[18:37] Dispensed 0.000517 mL of Base (0.5 M KOH)
[18:42] Stepping pH = 4.38
[18:42] Dispensed 0.000071 mL of Base (0.5 M KOH)
[18:47] Stepping pH = 4.37
[18:47] Dispensed 0.000376 mL of Base (0.5 M KOH)
[18:52] Stepping pH = 4.48
[19:07] Stirrer speed set to 0
[19:18] Datapoint id 12 collected
[19:18] Charge balance equation is out by 7.7%
[19:18] Stirrer speed set to 50
[19:23] pH 4.48 -> 4.68
[19:23] Using charge balance adjust
[19:23] Dispensed 0.001152 mL of Base (0.5 M KOH)
[19:43] Stirrer speed set to 0
[19:54] Datapoint id 13 collected
[19:54] Charge balance equation is out by 27.1%
[19:54] Stirrer speed set to 50
[19:59] pH 4.74 -> 4.94
[19:59] Using cautious pH adjust
[19:59] Dispensed 0.000541 mL of Base (0.5 M KOH)
[20:04] Stepping pH = 4.85
[20:05] Dispensed 0.000353 mL of Base (0.5 M KOH)
[20:10] Stepping pH = 4.90
[20:10] Dispensed 0.000212 mL of Base (0.5 M KOH)
[20:15] Stepping pH = 4.93
[20:15] Dispensed 0.000071 mL of Base (0.5 M KOH)
[20:20] Stepping pH = 4.93
[20:20] Dispensed 0.000165 mL of Base (0.5 M KOH)
[20:25] Stepping pH = 4.98
[20:40] Stirrer speed set to 0
[20:53] Datapoint id 14 collected
[20:53] Charge balance equation is out by -21.6%
[20:53] Stirrer speed set to 50
[20:58] pH 4.96 -> 5.16
[20:58] Using cautious pH adjust
[20:58] Dispensed 0.000470 mL of Base (0.5 M KOH)
[21:03] Stepping pH = 5.07
[21:03] Dispensed 0.000282 mL of Base (0.5 M KOH)
[21:08] Stepping pH = 5.12
[21:08] Dispensed 0.000188 mL of Base (0.5 M KOH)
[21:13] Stepping pH = 5.14
[21:13] Dispensed 0.000118 mL of Base (0.5 M KOH)
[21:19] Stepping pH = 5.15
[21:19] Dispensed 0.000118 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:24] Stepping pH = 5.18
[21:39] Stirrer speed set to 0
[21:52] Datapoint id 15 collected
[21:52] Charge balance equation is out by -25.4%
[21:52] Stirrer speed set to 50
[21:57] pH 5.17 -> 5.37
[21:57] Using cautious pH adjust
[21:58] Dispensed 0.000376 mL of Base (0.5 M KOH)
[22:03] Stepping pH = 5.30
[22:03] Dispensed 0.000141 mL of Base (0.5 M KOH)
[22:08] Stepping pH = 5.29
[22:08] Dispensed 0.000800 mL of Base (0.5 M KOH)
[22:13] Stepping pH = 5.59
[22:28] Stirrer speed set to 0
[22:46] Datapoint id 16 collected
[22:46] Charge balance equation is out by -79.4%
[22:46] Stirrer speed set to 50
[22:51] pH 5.54 -> 5.74
[22:51] Using cautious pH adjust
[22:51] Dispensed 0.000212 mL of Base (0.5 M KOH)
[22:56] Stepping pH = 5.57
[22:56] Dispensed 0.000494 mL of Base (0.5 M KOH)
[23:02] Stepping pH = 5.89
[23:17] Stirrer speed set to 0
[23:38] Datapoint id 17 collected
[23:38] Charge balance equation is out by -72.2%
[23:38] Stirrer speed set to 50
[23:43] pH 5.84 -> 6.04
[23:43] Using cautious pH adjust
[23:43] Dispensed 0.000118 mL of Base (0.5 M KOH)
[23:48] Stepping pH = 5.85
[23:48] Dispensed 0.000353 mL of Base (0.5 M KOH)
[23:53] Stepping pH = 6.29
[24:08] Stirrer speed set to 0
[24:33] Datapoint id 18 collected
[24:33] Charge balance equation is out by -89.2%
[24:33] Stirrer speed set to 50
[24:38] pH 6.26 -> 6.46
[24:38] Using cautious pH adjust
[24:38] Dispensed 0.000071 mL of Base (0.5 M KOH)
[24:44] Stepping pH = 6.26
[24:44] Dispensed 0.000188 mL of Base (0.5 M KOH)
[24:49] Stepping pH = 6.68
[25:04] Stirrer speed set to 0
[25:51] Datapoint id 19 collected
[25:51] Charge balance equation is out by -96.9%
[25:51] Stirrer speed set to 50
[25:57] pH 6.69 -> 6.89
[25:57] Using cautious pH adjust
[25:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:02] Stepping pH = 6.70
[26:02] Dispensed 0.000094 mL of Base (0.5 M KOH)
[26:07] Stepping pH = 6.87
[26:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:12] Stepping pH = 6.96
[26:27] Stirrer speed set to 0
[27:24] Datapoint id 20 collected
[27:24] Charge balance equation is out by -124.8%
[27:24] Stirrer speed set to 50

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[27:29] pH 7.02 -> 7.22
[27:29] Using cautious pH adjust
[27:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:34] Stepping pH = 7.04
[27:34] Dispensed 0.000047 mL of Base (0.5 M KOH)
[27:39] Stepping pH = 7.19
[27:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:44] Stepping pH = 7.38
[27:59] Stirrer speed set to 0
[28:59] Datapoint id 21 collected
[28:59] Charge balance equation is out by -161.1%
[28:59] Stirrer speed set to 50
[29:04] pH 7.46 -> 7.66
[29:04] Using cautious pH adjust
[29:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:09] Stepping pH = 7.49
[29:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:15] Stepping pH = 7.60
[29:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:20] Stepping pH = 7.84
[29:35] Stirrer speed set to 0
[30:35] Datapoint id 22 collected
[30:35] Charge balance equation is out by -351.4%
[30:35] Stirrer speed set to 50
[30:40] pH 7.98 -> 8.18
[30:40] Using cautious pH adjust
[30:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[30:45] Stepping pH = 8.02
[30:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[30:50] Stepping pH = 8.26
[31:05] Stirrer speed set to 0
[32:05] Datapoint id 23 collected
[32:05] Charge balance equation is out by -398.6%
[32:05] Stirrer speed set to 50
[32:10] pH 8.42 -> 8.62
[32:10] Using cautious pH adjust
[32:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:16] Stepping pH = 8.45
[32:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:21] Stepping pH = 8.64
[32:36] Stirrer speed set to 0
[33:19] Datapoint id 24 collected
[33:19] Charge balance equation is out by -209.9%
[33:19] Stirrer speed set to 50
[33:24] pH 8.71 -> 8.91
[33:24] Using cautious pH adjust
[33:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:29] Stepping pH = 8.73
[33:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:34] Stepping pH = 8.84
[33:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:39] Stepping pH = 8.98
[33:55] Stirrer speed set to 0
[34:23] Datapoint id 25 collected
[34:23] Charge balance equation is out by -216.2%
[34:23] Stirrer speed set to 50
[34:28] pH 9.01 -> 9.21
[34:28] Using cautious pH adjust
[34:28] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[34:33] Stepping pH = 9.01
[34:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[34:38] Stepping pH = 9.23
[34:53] Stirrer speed set to 0
[35:15] Datapoint id 26 collected
[35:15] Charge balance equation is out by -96.5%
[35:15] Stirrer speed set to 50
[35:20] pH 9.25 -> 9.45
[35:20] Using cautious pH adjust
[35:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:25] Stepping pH = 9.25
[35:25] Dispensed 0.000094 mL of Base (0.5 M KOH)
[35:30] Stepping pH = 9.48
[35:46] Stirrer speed set to 0
[36:04] Datapoint id 27 collected
[36:04] Charge balance equation is out by -96.5%
[36:04] Stirrer speed set to 50
[36:09] pH 9.49 -> 9.69
[36:09] Using cautious pH adjust
[36:09] Dispensed 0.000047 mL of Base (0.5 M KOH)
[36:14] Stepping pH = 9.51
[36:14] Dispensed 0.000141 mL of Base (0.5 M KOH)
[36:19] Stepping pH = 9.77
[36:34] Stirrer speed set to 0
[36:48] Datapoint id 28 collected
[36:48] Charge balance equation is out by -78.5%
[36:48] Stirrer speed set to 50
[36:53] pH 9.77 -> 9.97
[36:53] Using cautious pH adjust
[36:53] Dispensed 0.000094 mL of Base (0.5 M KOH)
[36:58] Stepping pH = 9.84
[36:58] Dispensed 0.000118 mL of Base (0.5 M KOH)
[37:03] Stepping pH = 9.96
[37:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:08] Stepping pH = 9.97
[37:23] Stirrer speed set to 0
[37:34] Datapoint id 29 collected
[37:34] Charge balance equation is out by -18.4%
[37:34] Stirrer speed set to 50
[37:39] pH 9.96 -> 10.05
[37:39] Using cautious pH adjust
[37:39] Dispensed 0.000047 mL of Base (0.5 M KOH)
[37:45] Stepping pH = 9.96
[37:45] Dispensed 0.000165 mL of Base (0.5 M KOH)
[37:50] Stepping pH = 10.10
[38:05] Stirrer speed set to 0
[38:15] Datapoint id 30 collected
[38:15] Charge balance equation is out by -90.3%
[38:15] Titration 2 of 3
[38:15] Adding initial titrants
[38:15] Automatically add 0.05000 mL of Octanol
[38:17] Dispensed 0.050000 mL of Octanol
[38:17] Stirrer speed set to 10
[38:18] Stirrer speed set to 55
[38:18] Iterative adjust 10.09 -> 2.00
[38:18] pH 10.09 -> 2.00
[38:19] Dispensed 0.054774 mL of Acid (0.5 M HCl)
[38:24] pH 2.01 -> 2.00
[38:24] Dispensed 0.001411 mL of Acid (0.5 M HCl)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[39:15] Stirrer speed set to 0
[39:25] Datapoint id 31 collected
[39:25] Stirrer speed set to 55
[39:30] pH 1.96 -> 2.16
[39:30] Using cautious pH adjust
[39:30] Dispensed 0.009337 mL of Base (0.5 M KOH)
[39:35] Stepping pH = 2.06
[39:35] Dispensed 0.005809 mL of Base (0.5 M KOH)
[39:41] Stepping pH = 2.13
[39:41] Dispensed 0.001881 mL of Base (0.5 M KOH)
[39:46] Stepping pH = 2.16
[40:01] Stirrer speed set to 0
[40:11] Datapoint id 32 collected
[40:11] Charge balance equation is out by 8.8%
[40:11] Stirrer speed set to 55
[40:16] pH 2.16 -> 2.36
[40:16] Using charge balance adjust
[40:16] Dispensed 0.011759 mL of Base (0.5 M KOH)
[40:37] Stirrer speed set to 0
[40:47] Datapoint id 33 collected
[40:47] Charge balance equation is out by 14.2%
[40:47] Stirrer speed set to 55
[40:52] pH 2.39 -> 2.59
[40:52] Using charge balance adjust
[40:53] Dispensed 0.006891 mL of Base (0.5 M KOH)
[41:13] Stirrer speed set to 0
[41:23] Datapoint id 34 collected
[41:23] Charge balance equation is out by 4.7%
[41:23] Stirrer speed set to 55
[41:28] pH 2.61 -> 2.81
[41:28] Using charge balance adjust
[41:28] Dispensed 0.004257 mL of Base (0.5 M KOH)
[41:48] Stirrer speed set to 0
[41:58] Datapoint id 35 collected
[41:58] Charge balance equation is out by 7.3%
[41:58] Stirrer speed set to 55
[42:03] pH 2.83 -> 3.03
[42:03] Using charge balance adjust
[42:03] Dispensed 0.002681 mL of Base (0.5 M KOH)
[42:24] Stirrer speed set to 0
[42:34] Datapoint id 36 collected
[42:34] Charge balance equation is out by 0.1%
[42:34] Stirrer speed set to 55
[42:39] pH 3.04 -> 3.24
[42:39] Using charge balance adjust
[42:39] Dispensed 0.001858 mL of Base (0.5 M KOH)
[42:59] Stirrer speed set to 0
[43:09] Datapoint id 37 collected
[43:09] Charge balance equation is out by -6.5%
[43:09] Stirrer speed set to 55
[43:14] pH 3.23 -> 3.43
[43:14] Using charge balance adjust
[43:14] Dispensed 0.001458 mL of Base (0.5 M KOH)
[43:35] Stirrer speed set to 0
[43:45] Datapoint id 38 collected
[43:45] Charge balance equation is out by 21.9%
[43:45] Stirrer speed set to 55
[43:50] pH 3.49 -> 3.69
[43:50] Using cautious pH adjust

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[43:50] Dispensed 0.000635 mL of Base (0.5 M KOH)
[43:55] Stepping pH = 3.64
[43:55] Dispensed 0.000165 mL of Base (0.5 M KOH)
[44:00] Stepping pH = 3.67
[44:00] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:05] Stepping pH = 3.68
[44:05] Dispensed 0.000094 mL of Base (0.5 M KOH)
[44:10] Stepping pH = 3.70
[44:25] Stirrer speed set to 0
[44:36] Datapoint id 39 collected
[44:36] Charge balance equation is out by 24.8%
[44:36] Stirrer speed set to 55
[44:41] pH 3.70 -> 3.90
[44:41] Using cautious pH adjust
[44:41] Dispensed 0.000635 mL of Base (0.5 M KOH)
[44:46] Stepping pH = 3.89
[45:01] Stirrer speed set to 0
[45:11] Datapoint id 40 collected
[45:11] Charge balance equation is out by 50.0%
[45:11] Stirrer speed set to 55
[45:16] pH 3.89 -> 4.09
[45:16] Using cautious pH adjust
[45:16] Dispensed 0.000635 mL of Base (0.5 M KOH)
[45:21] Stepping pH = 4.04
[45:21] Dispensed 0.000188 mL of Base (0.5 M KOH)
[45:26] Stepping pH = 4.08
[45:42] Stirrer speed set to 0
[45:52] Datapoint id 41 collected
[45:52] Charge balance equation is out by 35.8%
[45:52] Stirrer speed set to 55
[45:57] pH 4.08 -> 4.28
[45:57] Using cautious pH adjust
[45:57] Dispensed 0.000635 mL of Base (0.5 M KOH)
[46:02] Stepping pH = 4.22
[46:02] Dispensed 0.000235 mL of Base (0.5 M KOH)
[46:07] Stepping pH = 4.26
[46:07] Dispensed 0.000094 mL of Base (0.5 M KOH)
[46:12] Stepping pH = 4.27
[46:27] Stirrer speed set to 0
[46:37] Datapoint id 42 collected
[46:37] Charge balance equation is out by 24.0%
[46:37] Stirrer speed set to 55
[46:42] pH 4.27 -> 4.47
[46:42] Using cautious pH adjust
[46:43] Dispensed 0.000588 mL of Base (0.5 M KOH)
[46:48] Stepping pH = 4.40
[46:48] Dispensed 0.000282 mL of Base (0.5 M KOH)
[46:53] Stepping pH = 4.45
[46:53] Dispensed 0.000094 mL of Base (0.5 M KOH)
[46:58] Stepping pH = 4.46
[46:58] Dispensed 0.000118 mL of Base (0.5 M KOH)
[47:03] Stepping pH = 4.48
[47:18] Stirrer speed set to 0
[47:28] Datapoint id 43 collected
[47:28] Charge balance equation is out by 8.5%
[47:28] Stirrer speed set to 55
[47:33] pH 4.48 -> 4.68
[47:33] Using charge balance adjust
[47:33] Dispensed 0.000988 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[47:54] Stirrer speed set to 0
[48:04] Datapoint id 44 collected
[48:04] Charge balance equation is out by 3.3%
[48:04] Stirrer speed set to 55
[48:09] pH 4.70 -> 4.90
[48:09] Using charge balance adjust
[48:09] Dispensed 0.000753 mL of Base (0.5 M KOH)
[48:29] Stirrer speed set to 0
[48:40] Datapoint id 45 collected
[48:40] Charge balance equation is out by -14.9%
[48:40] Stirrer speed set to 55
[48:45] pH 4.88 -> 5.08
[48:45] Using charge balance adjust
[48:45] Dispensed 0.000564 mL of Base (0.5 M KOH)
[49:05] Stirrer speed set to 0
[49:16] Datapoint id 46 collected
[49:16] Charge balance equation is out by -25.1%
[49:16] Stirrer speed set to 55
[49:21] pH 5.05 -> 5.25
[49:21] Using cautious pH adjust
[49:21] Dispensed 0.000212 mL of Base (0.5 M KOH)
[49:26] Stepping pH = 5.10
[49:26] Dispensed 0.000329 mL of Base (0.5 M KOH)
[49:31] Stepping pH = 5.27
[49:47] Stirrer speed set to 0
[49:58] Datapoint id 47 collected
[49:58] Charge balance equation is out by -26.5%
[49:58] Stirrer speed set to 55
[50:03] pH 5.28 -> 5.48
[50:03] Using cautious pH adjust
[50:03] Dispensed 0.000141 mL of Base (0.5 M KOH)
[50:08] Stepping pH = 5.32
[50:08] Dispensed 0.000235 mL of Base (0.5 M KOH)
[50:13] Stepping pH = 5.50
[50:28] Stirrer speed set to 0
[50:40] Datapoint id 48 collected
[50:40] Charge balance equation is out by -34.5%
[50:40] Stirrer speed set to 55
[50:45] pH 5.52 -> 5.72
[50:45] Using cautious pH adjust
[50:45] Dispensed 0.000094 mL of Base (0.5 M KOH)
[50:50] Stepping pH = 5.55
[50:50] Dispensed 0.000165 mL of Base (0.5 M KOH)
[50:55] Stepping pH = 5.77
[51:10] Stirrer speed set to 0
[51:25] Datapoint id 49 collected
[51:25] Charge balance equation is out by -41.4%
[51:25] Stirrer speed set to 55
[51:30] pH 5.79 -> 5.99
[51:30] Using cautious pH adjust
[51:30] Dispensed 0.000071 mL of Base (0.5 M KOH)
[51:35] Stepping pH = 5.82
[51:35] Dispensed 0.000141 mL of Base (0.5 M KOH)
[51:40] Stepping pH = 6.15
[51:55] Stirrer speed set to 0
[52:15] Datapoint id 50 collected
[52:15] Charge balance equation is out by -59.1%
[52:15] Stirrer speed set to 55
[52:20] pH 6.18 -> 6.38

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[52:20] Using cautious pH adjust
[52:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[52:25] Stepping pH = 6.22
[52:25] Dispensed 0.000071 mL of Base (0.5 M KOH)
[52:30] Stepping pH = 6.55
[52:45] Stirrer speed set to 0
[53:37] Datapoint id 51 collected
[53:37] Charge balance equation is out by -52.2%
[53:37] Stirrer speed set to 55
[53:42] pH 6.63 -> 6.83
[53:42] Using cautious pH adjust
[53:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:47] Stepping pH = 6.64
[53:47] Dispensed 0.000071 mL of Base (0.5 M KOH)
[53:52] Stepping pH = 7.11
[54:07] Stirrer speed set to 0
[55:07] Datapoint id 52 collected
[55:07] Charge balance equation is out by -86.4%
[55:07] Stirrer speed set to 55
[55:13] pH 7.04 -> 7.24
[55:13] Using cautious pH adjust
[55:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:18] Stepping pH = 7.01
[55:18] Dispensed 0.000071 mL of Base (0.5 M KOH)
[55:23] Stepping pH = 7.76
[55:38] Stirrer speed set to 0
[56:38] Datapoint id 53 collected
[56:38] Charge balance equation is out by -279.5%
[56:38] Stirrer speed set to 55
[56:43] pH 7.97 -> 8.17
[56:43] Using cautious pH adjust
[56:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:48] Stepping pH = 8.01
[56:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:53] Stepping pH = 8.15
[56:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:58] Stepping pH = 8.29
[57:14] Stirrer speed set to 0
[58:14] Datapoint id 54 collected
[58:14] Charge balance equation is out by -699.4%
[58:14] Stirrer speed set to 55
[58:19] pH 8.07 -> 8.27
[58:19] Using cautious pH adjust
[58:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:24] Stepping pH = 8.04
[58:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:29] Stepping pH = 8.33
[58:44] Stirrer speed set to 0
[59:35] Datapoint id 55 collected
[59:35] Charge balance equation is out by -428.0%
[59:35] Stirrer speed set to 55
[59:40] pH 8.41 -> 8.61
[59:40] Using cautious pH adjust
[59:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:45] Stepping pH = 8.45
[59:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:50] Stepping pH = 8.56
[59:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:55] Stepping pH = 8.69

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:00:10] Stirrer speed set to 0
[1:00:48] Datapoint id 56 collected
[1:00:48] Charge balance equation is out by -357.1%
[1:00:48] Stirrer speed set to 55
[1:00:53] pH 8.73 -> 8.93
[1:00:53] Using cautious pH adjust
[1:00:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:59] Stepping pH = 8.73
[1:00:59] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:01:04] Stepping pH = 8.91
[1:01:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:09] Stepping pH = 8.99
[1:01:24] Stirrer speed set to 0
[1:01:53] Datapoint id 57 collected
[1:01:53] Charge balance equation is out by -204.7%
[1:01:53] Stirrer speed set to 55
[1:01:59] pH 9.00 -> 9.20
[1:01:59] Using cautious pH adjust
[1:01:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:04] Stepping pH = 8.99
[1:02:04] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:02:09] Stepping pH = 9.35
[1:02:24] Stirrer speed set to 0
[1:02:38] Datapoint id 58 collected
[1:02:38] Charge balance equation is out by -205.9%
[1:02:38] Stirrer speed set to 55
[1:02:44] pH 9.36 -> 9.56
[1:02:44] Using cautious pH adjust
[1:02:44] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:02:49] Stepping pH = 9.37
[1:02:49] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:02:54] Stepping pH = 9.58
[1:03:09] Stirrer speed set to 0
[1:03:25] Datapoint id 59 collected
[1:03:25] Charge balance equation is out by -88.1%
[1:03:25] Stirrer speed set to 55
[1:03:30] pH 9.57 -> 9.77
[1:03:30] Using cautious pH adjust
[1:03:30] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:03:35] Stepping pH = 9.61
[1:03:35] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:03:40] Stepping pH = 9.77
[1:03:55] Stirrer speed set to 0
[1:04:09] Datapoint id 60 collected
[1:04:09] Charge balance equation is out by -44.9%
[1:04:09] Stirrer speed set to 55
[1:04:14] pH 9.77 -> 9.97
[1:04:14] Using cautious pH adjust
[1:04:14] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:04:19] Stepping pH = 9.83
[1:04:19] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:04:24] Stepping pH = 9.93
[1:04:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:04:29] Stepping pH = 9.96
[1:04:44] Stirrer speed set to 0
[1:04:55] Datapoint id 61 collected
[1:04:55] Charge balance equation is out by -40.3%
[1:04:55] Stirrer speed set to 55
[1:05:00] pH 9.95 -> 10.05

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28012**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28012_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:05:00] Using cautious pH adjust
[1:05:00] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:05:05] Stepping pH = 9.98
[1:05:05] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:05:10] Stepping pH = 10.04
[1:05:25] Stirrer speed set to 0
[1:05:35] Datapoint id 62 collected
[1:05:35] Charge balance equation is out by -24.0%
[1:05:35] Titration 3 of 3
[1:05:35] Adding initial titrants
[1:05:35] Automatically add 0.25000 mL of Octanol
[1:05:41] Dispensed 0.250000 mL of Octanol
[1:05:41] Stirrer speed set to 10
[1:05:42] Stirrer speed set to 60
[1:05:42] Iterative adjust 10.05 -> 2.00
[1:05:42] pH 10.05 -> 2.00
[1:05:44] Dispensed 0.057714 mL of Acid (0.5 M HCl)
[1:05:49] pH 2.02 -> 2.00
[1:05:49] Dispensed 0.002587 mL of Acid (0.5 M HCl)
[1:06:39] Stirrer speed set to 0
[1:06:49] Datapoint id 63 collected
[1:06:49] Stirrer speed set to 60
[1:06:54] pH 1.96 -> 2.16
[1:06:54] Using cautious pH adjust
[1:06:55] Dispensed 0.010113 mL of Base (0.5 M KOH)
[1:07:00] Stepping pH = 2.05
[1:07:00] Dispensed 0.007620 mL of Base (0.5 M KOH)
[1:07:05] Stepping pH = 2.14
[1:07:05] Dispensed 0.001270 mL of Base (0.5 M KOH)
[1:07:10] Stepping pH = 2.16
[1:07:26] Stirrer speed set to 0
[1:07:36] Datapoint id 64 collected
[1:07:36] Charge balance equation is out by 6.0%
[1:07:36] Stirrer speed set to 60
[1:07:41] pH 2.17 -> 2.37
[1:07:41] Using charge balance adjust
[1:07:42] Dispensed 0.012512 mL of Base (0.5 M KOH)
[1:08:02] Stirrer speed set to 0
[1:08:12] Datapoint id 65 collected
[1:08:12] Charge balance equation is out by 7.3%
[1:08:12] Stirrer speed set to 60
[1:08:17] pH 2.39 -> 2.59
[1:08:17] Using charge balance adjust
[1:08:17] Dispensed 0.007620 mL of Base (0.5 M KOH)
[1:08:37] Stirrer speed set to 0
[1:08:47] Datapoint id 66 collected
[1:08:47] Charge balance equation is out by 11.9%
[1:08:47] Stirrer speed set to 60
[1:08:52] pH 2.62 -> 2.82
[1:08:52] Using charge balance adjust
[1:08:53] Dispensed 0.004704 mL of Base (0.5 M KOH)
[1:09:13] Stirrer speed set to 0
[1:09:23] Datapoint id 67 collected
[1:09:23] Charge balance equation is out by -2.4%
[1:09:23] Stirrer speed set to 60
[1:09:29] pH 2.82 -> 3.02
[1:09:29] Using charge balance adjust
[1:09:29] Dispensed 0.003269 mL of Base (0.5 M KOH)
[1:09:49] Stirrer speed set to 0

Sample name: **M07_octanol**
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Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:09:59] Datapoint id 68 collected
[1:09:59] Charge balance equation is out by 6.0%
[1:09:59] Stirrer speed set to 60
[1:10:04] pH 3.04 -> 3.24
[1:10:04] Using charge balance adjust
[1:10:04] Dispensed 0.002399 mL of Base (0.5 M KOH)
[1:10:24] Stirrer speed set to 0
[1:10:34] Datapoint id 69 collected
[1:10:34] Charge balance equation is out by 13.8%
[1:10:34] Stirrer speed set to 60
[1:10:40] pH 3.27 -> 3.47
[1:10:40] Using charge balance adjust
[1:10:40] Dispensed 0.001929 mL of Base (0.5 M KOH)
[1:11:00] Stirrer speed set to 0
[1:11:10] Datapoint id 70 collected
[1:11:10] Charge balance equation is out by 10.7%
[1:11:10] Stirrer speed set to 60
[1:11:15] pH 3.50 -> 3.70
[1:11:15] Using charge balance adjust
[1:11:15] Dispensed 0.001670 mL of Base (0.5 M KOH)
[1:11:35] Stirrer speed set to 0
[1:11:46] Datapoint id 71 collected
[1:11:46] Charge balance equation is out by 1.9%
[1:11:46] Stirrer speed set to 60
[1:11:51] pH 3.71 -> 3.91
[1:11:51] Using charge balance adjust
[1:11:51] Dispensed 0.001435 mL of Base (0.5 M KOH)
[1:12:11] Stirrer speed set to 0
[1:12:22] Datapoint id 72 collected
[1:12:22] Charge balance equation is out by -6.8%
[1:12:22] Stirrer speed set to 60
[1:12:27] pH 3.91 -> 4.11
[1:12:27] Using charge balance adjust
[1:12:27] Dispensed 0.001223 mL of Base (0.5 M KOH)
[1:12:47] Stirrer speed set to 0
[1:12:57] Datapoint id 73 collected
[1:12:57] Charge balance equation is out by 8.5%
[1:12:57] Stirrer speed set to 60
[1:13:02] pH 4.13 -> 4.33
[1:13:02] Using charge balance adjust
[1:13:03] Dispensed 0.000917 mL of Base (0.5 M KOH)
[1:13:23] Stirrer speed set to 0
[1:13:33] Datapoint id 74 collected
[1:13:33] Charge balance equation is out by 8.2%
[1:13:33] Stirrer speed set to 60
[1:13:38] pH 4.36 -> 4.56
[1:13:38] Using charge balance adjust
[1:13:38] Dispensed 0.000659 mL of Base (0.5 M KOH)
[1:13:58] Stirrer speed set to 0
[1:14:09] Datapoint id 75 collected
[1:14:09] Charge balance equation is out by 14.5%
[1:14:09] Stirrer speed set to 60
[1:14:14] pH 4.60 -> 4.80
[1:14:14] Using charge balance adjust
[1:14:14] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:14:35] Stirrer speed set to 0
[1:14:46] Datapoint id 76 collected
[1:14:46] Charge balance equation is out by 1.5%
[1:14:46] Stirrer speed set to 60

Sample name: **M07_octanol**
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Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:14:51] pH 4.82 -> 5.02
[1:14:51] Using charge balance adjust
[1:14:51] Dispensed 0.000282 mL of Base (0.5 M KOH)
[1:15:11] Stirrer speed set to 0
[1:15:22] Datapoint id 77 collected
[1:15:22] Charge balance equation is out by 6.9%
[1:15:22] Stirrer speed set to 60
[1:15:27] pH 5.04 -> 5.24
[1:15:27] Using charge balance adjust
[1:15:27] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:15:47] Stirrer speed set to 0
[1:15:59] Datapoint id 78 collected
[1:15:59] Charge balance equation is out by -32.4%
[1:15:59] Stirrer speed set to 60
[1:16:04] pH 5.20 -> 5.40
[1:16:04] Using cautious pH adjust
[1:16:04] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:16:09] Stepping pH = 5.23
[1:16:09] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:16:14] Stepping pH = 5.46
[1:16:29] Stirrer speed set to 0
[1:16:41] Datapoint id 79 collected
[1:16:41] Charge balance equation is out by -41.0%
[1:16:41] Stirrer speed set to 60
[1:16:46] pH 5.50 -> 5.70
[1:16:46] Using cautious pH adjust
[1:16:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:16:51] Stepping pH = 5.54
[1:16:51] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:16:56] Stepping pH = 5.75
[1:17:11] Stirrer speed set to 0
[1:17:35] Datapoint id 80 collected
[1:17:35] Charge balance equation is out by -44.5%
[1:17:35] Stirrer speed set to 60
[1:17:40] pH 5.82 -> 6.02
[1:17:40] Using cautious pH adjust
[1:17:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:17:45] Stepping pH = 5.83
[1:17:45] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:17:50] Stepping pH = 6.40
[1:18:05] Stirrer speed set to 0
[1:19:05] Datapoint id 81 collected
[1:19:05] Charge balance equation is out by -88.8%
[1:19:05] Stirrer speed set to 60
[1:19:10] pH 6.36 -> 6.56
[1:19:10] Using cautious pH adjust
[1:19:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:15] Stepping pH = 6.40
[1:19:15] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:19:20] Stepping pH = 6.66
[1:19:35] Stirrer speed set to 0
[1:20:35] Datapoint id 82 collected
[1:20:35] Charge balance equation is out by -45.8%
[1:20:35] Stirrer speed set to 60
[1:20:40] pH 6.67 -> 6.87
[1:20:40] Using cautious pH adjust
[1:20:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:45] Stepping pH = 6.70
[1:20:45] Dispensed 0.000047 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:20:51] Stepping pH = 7.15
[1:21:06] Stirrer speed set to 0
[1:22:06] Datapoint id 83 collected
[1:22:06] Charge balance equation is out by -73.9%
[1:22:06] Stirrer speed set to 60
[1:22:11] pH 7.13 -> 7.33
[1:22:11] Using cautious pH adjust
[1:22:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:16] Stepping pH = 7.19
[1:22:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:21] Stepping pH = 7.37
[1:22:36] Stirrer speed set to 0
[1:23:36] Datapoint id 84 collected
[1:23:36] Charge balance equation is out by -87.9%
[1:23:36] Stirrer speed set to 60
[1:23:41] pH 7.36 -> 7.56
[1:23:41] Using cautious pH adjust
[1:23:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:46] Stepping pH = 7.41
[1:23:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:52] Stepping pH = 7.71
[1:24:07] Stirrer speed set to 0
[1:25:07] Datapoint id 85 collected
[1:25:07] Charge balance equation is out by -173.4%
[1:25:07] Stirrer speed set to 60
[1:25:12] pH 7.90 -> 8.10
[1:25:12] Using cautious pH adjust
[1:25:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:17] Stepping pH = 7.97
[1:25:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:25:22] Stepping pH = 8.16
[1:25:37] Stirrer speed set to 0
[1:26:37] Datapoint id 86 collected
[1:26:37] Charge balance equation is out by -375.0%
[1:26:37] Stirrer speed set to 60
[1:26:42] pH 8.13 -> 8.33
[1:26:42] Using cautious pH adjust
[1:26:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:47] Stepping pH = 8.15
[1:26:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:53] Stepping pH = 8.23
[1:26:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:58] Stepping pH = 8.34
[1:27:13] Stirrer speed set to 0
[1:28:13] Datapoint id 87 collected
[1:28:13] Charge balance equation is out by -530.1%
[1:28:13] Stirrer speed set to 60
[1:28:18] pH 8.40 -> 8.60
[1:28:18] Using cautious pH adjust
[1:28:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:23] Stepping pH = 8.46
[1:28:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:28] Stepping pH = 8.56
[1:28:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:28:33] Stepping pH = 8.61
[1:28:48] Stirrer speed set to 0
[1:29:10] Datapoint id 88 collected
[1:29:10] Charge balance equation is out by -322.0%
[1:29:10] Stirrer speed set to 60

Sample name: **M07_octanol**
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Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:29:16] pH 8.63 -> 8.83
[1:29:16] Using cautious pH adjust
[1:29:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:21] Stepping pH = 8.66
[1:29:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:26] Stepping pH = 8.73
[1:29:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:31] Stepping pH = 8.80
[1:29:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:36] Stepping pH = 8.89
[1:29:51] Stirrer speed set to 0
[1:30:18] Datapoint id 89 collected
[1:30:18] Charge balance equation is out by -324.1%
[1:30:18] Stirrer speed set to 60
[1:30:23] pH 8.89 -> 9.09
[1:30:23] Using cautious pH adjust
[1:30:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:30:28] Stepping pH = 8.90
[1:30:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:30:34] Stepping pH = 9.01
[1:30:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:30:39] Stepping pH = 9.04
[1:30:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:30:44] Stepping pH = 9.09
[1:30:59] Stirrer speed set to 0
[1:31:14] Datapoint id 90 collected
[1:31:14] Charge balance equation is out by -257.9%
[1:31:14] Stirrer speed set to 60
[1:31:19] pH 9.11 -> 9.31
[1:31:19] Using cautious pH adjust
[1:31:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:24] Stepping pH = 9.12
[1:31:24] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:31:29] Stepping pH = 9.30
[1:31:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:34] Stepping pH = 9.32
[1:31:49] Stirrer speed set to 0
[1:32:01] Datapoint id 91 collected
[1:32:01] Charge balance equation is out by -124.8%
[1:32:01] Stirrer speed set to 60
[1:32:06] pH 9.31 -> 9.51
[1:32:06] Using cautious pH adjust
[1:32:06] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:32:11] Stepping pH = 9.35
[1:32:11] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:32:16] Stepping pH = 9.49
[1:32:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:21] Stepping pH = 9.50
[1:32:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:26] Stepping pH = 9.52
[1:32:41] Stirrer speed set to 0
[1:32:57] Datapoint id 92 collected
[1:32:57] Charge balance equation is out by -93.9%
[1:32:57] Stirrer speed set to 60
[1:33:02] pH 9.50 -> 9.70
[1:33:02] Using cautious pH adjust
[1:33:02] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:33:07] Stepping pH = 9.58
[1:33:07] Dispensed 0.000071 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
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Experiment start time: **2/28/2018 5:44:56 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:33:12] Stepping pH = 9.65
[1:33:12] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:33:17] Stepping pH = 9.68
[1:33:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:33:22] Stepping pH = 9.70
[1:33:37] Stirrer speed set to 0
[1:33:48] Datapoint id 93 collected
[1:33:48] Charge balance equation is out by -50.3%
[1:33:48] Stirrer speed set to 60
[1:33:53] pH 9.69 -> 9.89
[1:33:53] Using cautious pH adjust
[1:33:53] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:33:58] Stepping pH = 9.76
[1:33:58] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:34:03] Stepping pH = 9.85
[1:34:03] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:34:08] Stepping pH = 9.87
[1:34:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:14] Stepping pH = 9.89
[1:34:29] Stirrer speed set to 0
[1:34:40] Datapoint id 94 collected
[1:34:40] Charge balance equation is out by -41.2%
[1:34:40] Stirrer speed set to 60
[1:34:45] pH 9.89 -> 10.05
[1:34:45] Using cautious pH adjust
[1:34:45] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:34:50] Stepping pH = 9.94
[1:34:51] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:34:56] Stepping pH = 10.02
[1:35:11] Stirrer speed set to 0
[1:35:21] Datapoint id 95 collected
[1:35:21] Charge balance equation is out by -9.4%
[1:35:21] Argon flow rate set to 0
[1:35:25] Titrator arm moved over Titration position